

energy cost of mixing a solute in a solvent is reduced to a minimum. In this case, the solubility parameters of both solvent and solute are the same [11]. Indeed, exfoliation can occur when the net energy cost is very low. In chemistry, this energy balance is expressed by the enthalpy of the mixture (per unit of volume), which can be roughly calculated as [11]:

$$\frac{\Delta H_{mix}}{V_{mix}} \sim \frac{2}{T_{flake}} (\delta_G - \delta_{flake})^2 \phi \quad (1)$$

where H_{mix} is the enthalpy of the mixture, V_{mix} is the mixture volume, T_{flake} is the thickness of the flake, $\delta_i = \sqrt{E_{sur}^i}$ with E_{sur}^i the surface energy of i phase (where G indicates graphene bulk and $flake$ indicates graphene nanosheets respectively) and ϕ is the volume fraction of exfoliated material.

- *Size Selection*: the exfoliation of bulk materials in their 2D counterparts by LPE results in the production of an heterogeneous dispersion as concerns both the thickness and lateral size of the produced materials. Although this kind of dispersions is suitable for some applications (such as in the field of composite materials), for others this is not the best choice. In fact, the physico-chemical properties of 2D materials strongly depend on their morphology, so a size-selection step is needed [10]. In this work, a particular technique, based on (ultra) techniques centrifugation, will be discussed: the Sedimentation-Based Separation (SBS) [10]. SBS method allows the separation of nanomaterials based on their sedimentation rate, in response to a centrifugal force acting on them. In general, the rate of sedimentation of the dispersed materials subjected to a centrifugal field is described by the Svedberg equation [10]:

$$S = \frac{1 - \rho v}{f} \quad (2)$$

where S is the sedimentation coefficient (the time required for the nanomaterial to sediment), m is the mass of the flake, ρ is the solvent density, v is the volume that each gram of nanoparticles or nanosheets occupies in solution, and f is the friction coefficient [10]. Overall, the sedimentation coefficient depends on the morphological properties of the displaced nanomaterial and is proportional to its actual molar weight, while it is inversely proportional to f . The thicker and larger flakes, which have a greater mass, settle faster than small and thin flakes (with lower mass), which are thus held in dispersion during a SBS process (Fig. 1) [10].

Raman characterization of TMDCs

Once the 2D material is prepared, it is necessary to assess physico-chemical properties such as structure, morphology, etc. An ideal characterization tool should be fast and non-destructive, with high spectral and spatial resolution, and be applicable in both laboratory and industrial scale. Raman spectroscopy is one of the most used techniques

to assess the structural and morphological properties of 2D materials. In fact, it can easily identify defects, structural damage, presence and status of functional groups, chemical modifications and electronic perturbations introduced during the preparation, processing or placement of the material [12]. For a proper interpretation of 2D materials Raman spectra, a thorough understanding of the material vibrational modes is pivotal. Lattice vibrations can be classified basing on the irreducible representation of the symmetry group of the crystals. The unit cell of bulk MX_2 consists of two X-M-X units with a total six atoms, suggesting that there are 18 phonon modes (3 acoustic and 15 optical modes). Bulk MX_2 has D_{6h} point group symmetry [13]. Thus, the lattice vibrations of bulk MX_2 at the Γ can be expressed by the irreducible representations of D_{6h} as follows [13]:

$$\Gamma = A_{1g} + 2A_{2u} + 2B_{2g} + B_{1u} + E_{1g} + 2E_{1u} + 2E_{2g} + E_{2u} \quad (3)$$

where one A_{2u} and one E_{1u} are acoustic modes; A_{1g} , E_{1g} and E_{2g} are Raman (R) active; another A_{2u} and E_{1u} are infrared (IR) active; B_{2g} , B_{1u} and E_{2u} are optically inactive (silent). Here the modes denoted by the letter ‘‘E’’ are doubly degenerate in the xy plane [13].

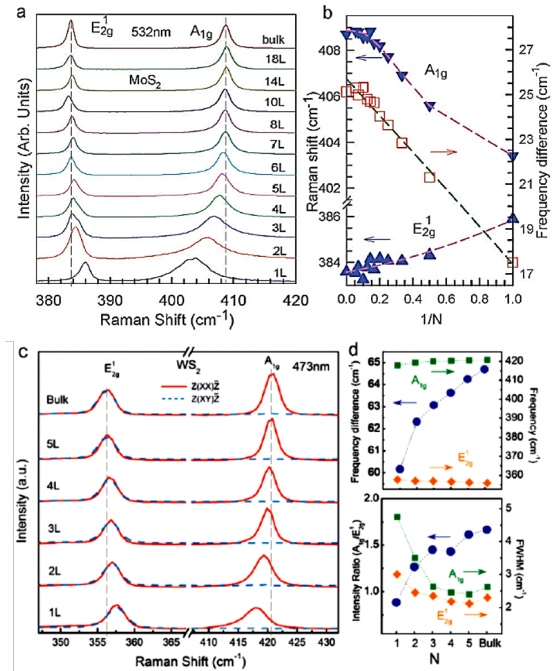


Figure 3: (a) Raman spectra of NL- and bulk MoS_2 . (b) Frequency and frequency difference between modes E_{2g}^1 and A_{1g} as a function of $1/N$ of MoS_2 . (c) Polarized Raman spectra of 1–5L and bulk WS_2 , with the frequencies of E_{2g}^1 and A_{1g} frequency difference, $I(A_{1g})/I(E_{2g}^1)$ and peak width summarized in (d) [13].

Because of the lack of translational symmetry (t) along the z axis which is perpendicular to the basal xy plane, there is a reduction in symmetry in $NL-MX_2$ (where N

indicates the number of layers while L indicates "layers"). Odd $NL-MX_2$ ($ONL-MX_2$, O indicates odd) has D_{3h} point group symmetry because of the presence of the horizontal reflection plane that passes through the transition metal atom (M). In particular, the unit cell of $1L-MX_2$ is composed of three atoms with nine normal vibrational modes at the point Γ , which is expressed based on D_{3h} as [13]:

$$\Gamma = 2A_2'' + A_1' + 2E' + E'' \quad (4)$$

where one A_2'' and one E' are acoustic modes, another A_{12} is IR active, A_1' and E'' are R active, and another E' is both R and IR active. The point group of even $NL-MX_2$ ($ENL-MX_2$) is D_{3d} because of the existence of inversion symmetry i [13]. σ_h exists in $ONL-MX_2$ and bulk MX_2 bulk but it is not present in $ENL-MX_2$. In particular, for $2L-MX_2$, the unit cell is composed of six atoms belonging to D_2 . There are 18 normal vibrational modes at the Γ point [13]:

$$\Gamma = 3A_{1g} + 3A_{2u} + 3E_g + 3E_u \quad (5)$$

where one A_{2u} and one E_u are acoustic modes; the other A_{2u} and E_u are IR active, and A_{1g} and E_g are R active [13]. The Raman measurements of MoS_2 (Fig. 3a-b) showed that the Raman contribution for the $E_{2g}^1(\Gamma)$ mode (due to the shift in the plane of the Mo atoms) is at higher frequencies for the flakes, compared to the contribution in the bulk case. This frequency shift for the $E_{2g}^1(\Gamma)$ mode is due to intra-layer bonds, which contribute to phononic modes. This does not happen instead for the $A_g^1(\Gamma)$ mode (associated with the displacement out of the plane of the S atoms), for which the Raman contribution remains unchanged, compared to the bulk of the MoS_2 , since the exfoliated material appears to be composed of several layers. Similar results were obtained for the WS_2 system (Fig. 3c). In this case is found a blue-shift, as a consequence of the decrease in the thickness of the WS_2 flakes (Fig. 3c)[13].

Conclusion

Two-dimensional materials have extraordinary physical properties, that make them ideal for several technological applications. The appropriate choice of the technique for the production of 2D materials and the structural characterization of products obtained are two fundamental steps for the realization of 2D systems of high quality. In this contribution, the Liquid Phase Exfoliation process has been described as a very efficient technique for the production of high quality 2D materials with low costs. Furthermore the phonon structure of MoS_2 and WS_2 dichalcogenides compounds and the capability of Raman spectroscopy to investigate their properties have been reviewed. In particular, it is shown that by analyzing the frequency separation between the peaks related to E_{2g}^1 and A_{1g} modes, information on the layer number of the MoS_2 and WS_2 systems can be obtained.

References

[1] ASHCROFT: "(Solid State Physics) Neil W."

- [2] A. C. FERRARI ET AL.: "Science and technology roadmap for graphene, related two-dimensional crystals, and hybrid systems" *Nanoscale*, vol. 7, no. 11, pp. 4598–4810, 2015.
- [3] A. A. BALANDIN: "Thermal properties of graphene and nanostructured carbon materials" *Nat. Mater.*, vol. 10, no. 8, pp. 569–581, 2011.
- [4] T. POLICHETTI ET. AL.: "Overview on graphene" *Chemistry Today*, vol. 28, no. December, pp. 6–9, 2010.
- [5] Q. H. WANG ET. AL.: "Electronics and optoelectronics of two-dimensional transition metal dichalcogenides" *Nat. Nanotechnol.*, vol. 7, no. 11, pp. 699–712, 2012.
- [6] S. MANZELI, D. OVCHINNIKOV, D. PASQUIER, O. V. YAZYEV, AND A. KIS: "2D transition metal dichalcogenides" *Nat. Rev. Mater.*, vol. 2, 2017.
- [7] Y. XU, H. CAO, Y. XUE, B. LI, AND W. CAI: "Liquid-phase exfoliation of graphene: An overview on exfoliation media, techniques, and challenges" *Nanomaterials*, vol. 8, no. 11, 2018.
- [8] L.W.T. NG ET AL.: "Printing of graphene and related 2D materials: Technology, formulation and applications" 2018.
- [9] M. YI AND Z. SHEN: "A review on mechanical exfoliation for the scalable production of graphene" *J. Mater. Chem. A*, vol. 3, no. 22, pp. 11700–11715, 2015.
- [10] F. BONACCORSO, A. BARTOLOTTA, J. N. COLEMAN, AND C. BACKES: "2D-Crystal-Based Functional Inks" *Adv. Mater.*, pp. 6136–6166, 2016.
- [11] Y. HERNANDEZ ET AL., "HERNANDEZ ET AL: "High yield production of graphene by liquid phase exfoliation of graphite" pp. 1–14.
- [12] J. N. COLEMAN: "Liquid exfoliation of defect-free graphene" *Acc. Chem. Res.*, vol. 46, no. 1, pp. 14–22, 2013.
- [13] X. ZHANG, X. F. QIAO, W. SHI, J. BIN WU, D. S. JIANG, AND P. H. TAN: "Phonon and Raman scattering of two-dimensional transition metal dichalcogenides from monolayer, multilayer to bulk material" *Chem. Soc. Rev.*, vol. 44, no. 9, pp. 2757–2785, 2015.

Acknowledgements

I thank Professor D'Angelo for following me in this thesis work. I thank the IPCF-CNR of Messina for allowing me to use their facilities. I thank the Graphene Labs of IIT, Genova, for providing me with the studied samples and some data.

Principles of a neuron-glia tripartite synapse based biomorphic processing unit

R. Musotto^{1-3,*}, M. De Pittà², G. Pioggia³

¹*University of Messina, Department of Physics, Messina, Italy*

²*University of the Basque Country, Basque center for applied mathematics, Bilbao, Spain.*

³*National Research Council of Italy (CNR), Institute for Biomedical Research and Innovation (IRIB), Messina, Italy*

*Corresponding Author email: rosy.musotto@libero.it

Abstract

Experimental evidence shows how astrocytes may be players in brain information processing, even if it is yet not understood how these cells could encode synaptic stimuli and influence the neuronal spiking activity. In this paper two aspects are considered: how calcium signalling in the astrocyte could integrate and encode synaptic stimuli and how astrocytes could affect information processing of neuronal activity. We describe the concept of tripartite synapse which describes the tight interactions between synaptic terminals and their surrounding astrocytic processes, and introduce models potentially able to define a biomorphic neuron model for a step-forward hardware-based neural network based on tripartite synapses.

Keywords: astrocytes, tripartite synapse, neuro-glia processing unit.

Introduction

In recent decades, emerging evidence are reporting how glial function deficits seem to be involved with neurological diseases, such as cerebral cortex, midbrain, and spinal cord, ataxias, developmental disorders, autism attention deficits, hyperactivity, schizophrenia, as well as neuroendocrine disorders and pediatric tumors [1]. Glial cell of the central nervous system (CNS) can be distinguished into four subtypes: microglia are the resident macrophages of the brain, oligodendrocytes serve a myelination role, glial neuroprogenitors give rise to the neurons of the brain, and astrocytes. Apart glia, studying neurons, usually researchers and clinicians refer to the term “neural code” thinking about to the properties of a single sequence of action potentials (spike trains) or a spike train ensemble to encode, decode, and process sensory and/or cognitive information. Is it possible to think of an analogous code for glial cells? [2]. Although astrocytes are not electrically excitable cells, namely they cannot generate action potentials, they possess a form of chemical excitability based on variations of their intracellular calcium concentration. These Ca²⁺ variations can be transient or oscillatory and can occur spontaneously or be induced by different means such as for example, by mechanical, electrical or chemical stimulation. In particular, astrocyte Ca²⁺ elevations can be elicited in response to a variety of neurotransmitters and factors including glutamate, GABA, adrenaline, ATP, serotonin, acetylcholine, dopamine, nitric oxide (Bergmann glia) and BDNF1. Such a response is mediated by different receptors localized on the astrocyte plasma membrane and

is usually consistent with the mobilization of Ca²⁺ from the intracellular stores of the endoplasmic reticulum.

The presence of receptors on astrocytes could be seen as the teleological evidence for neuron-to-glia signalling [2]. Among the possible glial codes, calcium signalling is the most studied one, arguably because of the availability of indicators to monitor intracellular Ca²⁺ [3], as well as for its recognized function as intracellular messenger in a multitude of other cells [4]. There are nonetheless further reasons why Ca²⁺ signalling could be an effective code for glial cells. In particular, Ca²⁺ signalling could serve all the four key functions originally proposed by Perkel and Bullock for a candidate neural code: stimulus representation, interpretation, transformation, and transmission [5]. Thus, astrocyte may affect the synapses in terms of information processing. Synapses play a critical role in processing information in the brain. They are involved in learning, short-term and long-term memory functions, temporal information processing, as well as signal transduction and plasticity of the brain. Proper synapse formation during childhood provides a substrate for cognition, whereas improper formation or functionality leads to neuro-developmental disorders including mental retardation and autism [6]. Our study pursued two main goals: (1) to investigate the possible factors that could underlie astrocyte to integrate and encode synaptic stimuli, and (2) to characterize elements could affect information processing of neuronal activity and the impact of astrocytic Ca²⁺ signals in terms of information processing performed by a tripartite synapse. A biomorphic neuron model may introduce conceptual principles of an hardware-based neural network connecting single tripartite synapse chips able to implement ultra-large neural

networks which in turn may simulate the operations of cortical column or areas in the stand-alone hardware.

The Human Brain

The human brain is a remarkable information storage and processing system. It possesses an extraordinary computation-per-volume efficiency, with an average weight of 1400 g and a volume of $\sim 1,350 \text{ cm}^3$, contained within an average intracranial volume of $\sim 1.7 \text{ cm}^3$ [7]. The brain in numbers can be summarized as: $\sim 1,350 \text{ cm}^3$ (75%) brain cells, $\sim 200 \text{ cm}^3$ (15%) blood, and up to $\sim 150 \text{ cm}^3$ (10%) of cerebrospinal fluid. The raw computational power of the human brain has been estimated to range from 10^{13} to 10^{16} operations/sec [8]. The human brain's functional action potential based information is estimated as 5.52×10^{16} bits/sec [9], with a brain power output estimated at 15–25 W and a power density of $1.1 - 1.8 \times 10^4 \text{ W/m}^3$ at an operating temperature of 37.3C [10]. The average human brain is estimated to contain $(86.06 \pm 8.2) \times 10^9$ neurons, with $\sim 80.2\%$ ($69.03 \pm 6.65 \times 10^9$ neurons) located in the cerebellum, $\sim 19\%$ ($16.34 \pm 2.17 \times 10^9$ neurons) located in the cerebral cortex, and only $\sim 0.8\%$ ($0.69 \pm 0.12 \times 10^9$ neurons) located throughout the rest of the brain. The human cerebellum and cerebral cortex together hold the vast majority (99.2%) of brain neurons [7]. The average number of glial cells in the human brain is estimated to be $84.61 \pm 9.83 \times 10^9$, with the population of glial cells in the neocortex estimated at from 18.2 to 38.6×10^9 [7]. The ratio of glia to neurons likely has functional relevance and varies between different brain regions. While the whole-brain glia/neuron ratio is $\sim 1:1$, there are significant differences between brain domains. For example, the glia/neuron ratio of the cerebral cortex is 3.72:1 (60.84 billion glia; 16.34 billion neurons) but only 0.23:1 (16.04 billion glia; 69.03 billion neurons) in the cerebellum; the basal ganglia, diencephalon, and brainstem have a combined ratio of 11.35:1 [11]. In addition, synapses, numbering $(2.42 \pm 0.29) \times 10^{14}$ in the average human brain, are collectively estimated to process information at spiking rates of $(4.31 \pm 0.86) \times 10^{15}$ spikes/sec, empowering the human brain to process data at $(5.52 \pm 1.13) \times 10^{16}$ bits/sec [7].

The novel "tripartite synapse" concept as a single processing unit

Several experiments indicated that Ca^{2+} signals in response to external stimulus can encode information via frequency modulation (FM) or in some other cases via amplitude modulation (AM) [12]. Our hypothesis is that, among other possibilities however, we may recognize a single tripartite (three-part) synapse processing unit involving a pre-synaptic neuron releasing neurotransmitters (glutamate) which activates or inhibits the activity of a post-synaptic neuron, the post-synaptic neuron and one

astrocyte which modulates glutamate in frequency and amplitude. This unit should represent a common denominator of a novel fundamental role of astrocytes in information processing of the brain. Based on previous works of authors and the state-of-the-art, our work can be strengthened by the calcium signalling in astrocytes, which is a predominant non-neuronal (glial) cell type that plays a crucial role in the regulation of neuronal activity. From a physiological point of view, astrocytes regulate the synaptic signalling current between two neurons modulating the amount of neurotransmitters into the synaptic cleft through inter- and intracellular calcium dynamics [2]. In detail, calcium dynamics is controlled by the interplay of calcium-induced calcium release, a nonlinear amplification method triggering the modulation of the pre-synaptic and post-synaptic neural activities and promoting depolarizing currents in neurons [13]. The interplay of calcium-induced calcium release nonlinear amplification method is dependent on calcium channels opening to calcium stores such as the endoplasmic reticulum, and the action of active transporters that enable a reverse flux [13,12]. The level of inositol 1, 4, 5-trisphosphate (IP3) is directly controlled by signals impinging on the cell from its external environment. The elevation of the intracellular calcium level in astrocytes, promoted by the extracellular glutamate, triggers the release of glutamate from the astrocyte, modulating the pre-synaptic and post-synaptic depolarizing currents in neurons. Furthermore, inositol 1, 4, 5-trisphosphate dynamics are encoded by nonlinear amplitude and frequency modulation phenomena, while calcium oscillations are inherently frequency modulated. The properties of Ca^{2+} oscillations generated in astrocytes such as their amplitude, frequency and propagation, are governed by the intrinsic properties of both these cells and those of neuronal inputs. Low-intensity synaptic stimulation and spontaneous astrocyte activity usually give rise to Ca^{2+} transients confined in small regions at the very end of distal processes which in Bergmann glia are also morphologically correlated with the microdomains observed in these cells. Such compartmentalization of Ca^{2+} signaling supports the hypothesis that subcellular portions of astrocytes could operate as independent functional units. On the contrary, high-intensity synaptic activity or concurrent stimulation of several synapses, consistent with the activation of adjacent sites of the same astrocytic process, are generally associated with Ca^{2+} elevations that propagate along the process in a form akin to that of regenerative Ca^{2+} waves. Such waves can be either intracellular, when they remain confined within the same astrocyte, or intercellular when they propagate from one cell to neighboring astrocytes. The frequency of astrocytic Ca^{2+} oscillations is likely to encode the level of synaptic activity [2]. Increases in frequency or intensity of synaptic stimulation result in fact in a corresponding increase in the frequency of Ca^{2+} oscillations. Notwithstanding, it is very likely that encoding of synaptic activity in the astrocyte Ca^{2+} signal could occur in a more complex fashion. Ca^{2+} oscillations indeed, can be highly variable in amplitude and their dynamics does not simply reflect synaptic activity. In this regard recent experimental findings showed that hippocampal as-

trocytes in situ can discriminate among neuronal inputs of different origins, namely of different axon pathways, and can also integrate concomitant inputs. In spite of these large amount of evidences astrocyte Ca^{2+} increases evoked by neuronal activity might be written off as a curious epiphenomenon of minor importance to brain function if it were not for the fact that they initiate additional astrocyte responses. Perhaps the most significant of these Ca^{2+} -dependent responses is the release of gliotransmitters from astrocytes. In order to implement a single and efficient processing unit, it is our aim to define a computational simple model of the tripartite synapse (both for neurons and the astrocyte) able to drive spiking in FM and/or AM or both, capturing the above-mentioned observations. It is worth mentioning that it was also shown that higher-order models with several dynamical variables and/or intracellular diffusion mechanisms can exhibit different and more advanced encoding modes. Considering how calcium dynamics is controlled by the interplay of calcium-induced calcium release, a nonlinear amplification process regulated by the calcium-dependent opening of channels to Ca^{2+} stores, the minimal model consisting of two dynamical variables such as the Li-Rinzel (LR) [2] may be effectively used in our unit. The two dynamical variables of LR model are the free cytosolic Ca^{2+} concentration (C), and the fraction of open inositol trisphosphate (IP3) receptor subunits, h ,

$$\begin{aligned}\dot{C} &= j_{chan}(C, I) + j_{leak}(C) - j_{pump}(C) \\ \dot{h} &= \frac{h_{\infty} h}{T_h}\end{aligned}$$

The dynamics of C is controlled by three fluxes, corresponding to (1) a passive leak of Ca^{2+} from the endoplasmic-reticulum (ER) of the cell to the cytosol (J_{leak}); (2) an active uptake of Ca^{2+} into ER, J_{pump} , due to the action of the pumps; (3) a Ca^{2+} release (J_{chan}) that is mutually gated by Ca^{2+} and the inositol trisphosphate (IP3) concentration (I),

$$J_{leak}(C) = v_2[C_0 - (1 + C_1)C],$$

$$J_{pump}(C) = \frac{v_3 C^2}{K_3^2 + C^2},$$

$$J_{chan}(C, I) = V_1 m^3 h^3 [C_0 - (1 + c_1)C].$$

The gating variables and their time scales are given by

$$C m_{\infty} = \frac{I}{I + d_1},$$

$$h_{\infty} = \frac{Q_2}{Q_2 + C},$$

$$T_h = \frac{1}{a_2(Q_2 + C)},$$

$$Q_2 = \frac{I + d_1}{I + d_3} d_2$$

The level of IP is directly controlled by signals impinging on the cell from its external environment. In turn, the level of IP3 determines the dynamical behavior of the above model. One can therefore think of the Ca^{2+} signal as being an encoding of information regarding the level of IP3. Thus, the level of IP3 is directly controlled by signals impinging on the cell from its external environment. In turn, the level of IP3 determines the dynamical behavior of the LR model. One can therefore consider the calcium signal as an encoded information regarding the level of IP3. In detail, by varying two key parameters of the model, the information can be encoded in amplitude or in frequency modulations of the calcium. These findings were recently demonstrated by De Pitta' et al. (2008) [12] and largely discussed in De Pittà and H. Berry (2019) [2]. The elevation of the intracellular calcium level in astrocytes, promoted by the extracellular glutamate, triggers the release of glutamate from the astrocyte modulating the pre-synaptic and post-synaptic neural activities by promoting a depolarizing current in neurons (Iastro). Regarding the pre- and post-synaptic neurons, we can adopt the artificial cortical neuron model proposed by Izhikevich [14]. It consists of two equations and a few several parameters:

$$\begin{cases} C v' = k(v - v_r)(v - v_t) - u + I_n \\ u' = a[b(v - v_r) - u] \end{cases}$$

C	100pF	a	0,03
K	0,7	b	-2
V_r	-60mV	c	-50mV
V_t	-40mV	d	100
V_{peak}	35mV		

When a neuron fires, it releases quantal amounts of neurotransmitters (glutamate) into the synaptic cleft. Neurotransmitters bind to the glutamate receptors on the astrocytes, triggering the release of intracellular IP3. In our computational model the modulation coming from an astrocyte can be modified as:

$$\begin{cases} C v' = k(v - v_r)(v - v_t) - u + I_n + I_{astro} \\ u' = a[b(v - v_r) - u] \end{cases}$$

I_{astro} represents the contribution of the astrocyte in terms of modulation current toward the post-synaptic neuron.

We are working to complete the model linking between calcium concentration and Iastro by means of experimental data. Our aim to implement an efficient firmware incorporating the above-mentioned models and the experimental data for a biomorphic chip able to embody the tripartite synapse processing unit in silico.

Discussion and Conclusions

The discovery of the existence of a bidirectional communication between astrocytes and neurons gave birth to the concept that synapses are probably tripartite structures. Therefore, synapses in the CNS are not merely constituted by a pre- and a postsynaptic terminal, but

rather they include a third element, the astrocyte, which represents an integral modulatory component of synaptic transmission. The implications from a functional point of view of a revisiting of synaptic transmission in terms of tripartite synapses are likely to be deep and not wholly appreciated at our current level of knowledge. Considering that a single astrocyte can cover $\sim 140\,000$ synapses, and that each microdomain ensheathes an average of 3–5 synapses, an astrocyte could be coupled with thousands of microdomains of tripartite synapses that could be independently modulated and/or synchronized by means of Ca^{2+} signalling and gliotransmitter release. Furthermore, differential synaptic stimulation could rise intercellular Ca^{2+} waves which could modulate synaptic transmission over long distances by releasing gliotransmitter at synapses far from those that were initially active. This mechanism suggests an additional role for astrocytes as mediators of heterosynaptic lateral information transfer. At last, synaptic modulation by astrocytes is probably coupled with blood flow and neural metabolism providing a further extension for the multiple effects of neuron-astrocyte communication in the physiology of the brain. Among all these possibilities however, we may recognize as a common denominator a novel fundamental role of astrocytes in information processing of the brain. Nonetheless it is difficult to imagine brain functions in terms of astrocytic signalling if we consider that the timescale of Ca^{2+} variations is slower than neuronal firing by six orders of magnitude and the timescale of gliotransmitter modulatory effects at synapses ranges between hundreds of milliseconds and minutes or even tens of minutes. Hence in order to address what roles astrocyte feedbacks on synaptic transmission could play as well as how they could influence the neuronal code, we consider the case of a glutamatergic tripartite synapse only, which is currently the best characterized experimental frame in the context of neuron-glia interactions. One of the original motivations of our work is the extremely complex experimental observations that Ca^{2+} oscillations in astrocytes should be modelled and implemented *in silico* by programming a biomorphic chip in terms of amplitude and frequency modulation of the synaptic activity to encode the spiking output of each single processing unit. In spite of our distinction between AM-encoding and FM-encoding, the emerging view is that Ca^{2+} signals use both these modes to encode information. The existence of such “AFM-encoding” in astrocytes remains currently elusive due to inherent limits of the available experimental techniques.

References

[1] Ana Paula Bergamo Araujo, Raul Carpi-Santos, Flávia Carvalho Alcantara Gomes: The Role of Astrocytes in the Development of the Cerebellum, *The Cerebellum* (2019) 18:1017–1035.

[2] M. De Pittà and H. Berry (eds.), *Computational Glioscience*, Springer Series in Computational Neuroscience, https://doi.org/10.1007/978-3-030-00817-8_1.

[3] Rusakov DA: Disentangling calcium-driven astrocyte physiology. *Nat Rev Neurosci* 16:226–233 (2015).

[4] Berridge MJ, Lipp P, Bootman MD: The versatility and universality of calcium signalling. *Nat Rev Mol Cell Biol* 1:11–21 (2000).

[5] Perkel DH, Bullock TH: Neural coding: a report based on an NRP work session. *Neurosci Res Program Bull* 6:219–349 (1968).

[6] Rollenhagen, A., and Lübke, J. H.: The morphology of excitatory central synapses: from structure to function. *Cell Tissue Res.* 326, 221–237. doi: 10.1007/s00441-006-0288-z. (2006).

[7] Martins NRB, Angelica A, Chakravarthy K, Svidnenko Y, Boehm FJ, Opris I, Lebedev MA, Swan M, Garan SA, Rosenfeld JV, Hogg T and Freitas RA Jr: Human Brain/Cloud Interface. *Front. Neurosci.* 13:112. doi: 10.3389/fnins.2019.00112 (2019).

[8] Merkle, R.: *Energy Limits to the Computational Power of the Human Brain*. Palo Alto, CA: Foresight Institute) (1989).

[9] Martins, N. R. B, Erlhagen, W., and Freitas, R. A. Jr.: Non-destructive whole-brain monitoring using nanorobots: neural electrical data rate requirements. *Int. J. Mach. Conscious.* 4, 109–140. doi: 10.1142/S1793843012400069 (2012).

[10] Freitas, R. A. Jr.: *Nanomedicine, Volume I: Basic Capabilities*. Georgetown, TX: Landes Bioscience (1999b).

[11] Azevedo, F. A., Carvalho, L. R., Grinberg, L. T., Farfel, J. M., Ferretti, R. E., Leite, R. E., et al.: Equal numbers of neuronal and nonneuronal cells make the human brain an isometrically scaled-up primate brain. *J. Comp. Neurol.* 513, 532–541. doi: 10.1002/cne. 2197 (2009).

[12] De Pittà M, Volman V, Levine H, Pioggia G, De Rossi D, Ben-Jacob E: Coexistence of amplitude and frequency modulations in intracellular calcium dynamics. *Phys Rev E* 77(3):030903(R) (2008).

[13] De Pittà M, Goldberg M, Volman V, Berry H, Ben-Jacob E: Glutamate-dependent intracellular calcium and IP_3 oscillating and pulsating dynamics in astrocytes. *J Biol Phys* 35:383–411 (2009).

[14] G. Valenza, G. Pioggia, A. Armato, M. Ferro, E.P. Scilingo, D. De Rossi: A neuron-astrocyte transistor-like model for neuromorphic dressed neurons, *Neural Networks* 24 (2011) 679–685

Eco-friendly Gas Mixtures for the Resistive Plate Chambers of the ALICE Muon Spectrometer

A. Rosano^{1,*}, A. Ferretti², A. Bianchi²

¹*Dipartimento di Scienze Matematiche e Informatiche, Scienze Fisiche e Scienze della Terra, Università degli Studi di Messina, viale F. Stagno d'Alcontres 31, Messina, Italy, and INFN, Sezione di Catania*

²*Dipartimento di Fisica, Università degli Studi di Torino, Via Pietro Giuria 1, Torino, Italy, and INFN, Sezione di Torino*

*Corresponding Author email: antonina_rosano@libero.it

Abstract

Single-gap Resistive Plate Chambers are gaseous detectors which deliver the muon trigger of the ALICE experiment. The gas mixture is made of $C_2H_2F_4$, SF_6 and $i-C_4H_{10}$. Since the first two gases have high Global Warming Potentials, it is essential to find a new eco-friendly gas mixture, both to reduce greenhouse gases emission and to deal with their price increase, due to EU restrictions. In this work will be shown results obtained by testing a $50 \times 50 \text{ cm}^2$ RPC, exposed to cosmic rays and fluxed with gas mixtures containing different $C_3H_2F_4 + CO_2$ concentrations in place of $C_2H_2F_4$. Furthermore $i-C_4H_{10}$ and SF_6 quenching effects in the new gas mixtures have been also explored.

Keywords: Resistive Plate Chambers, ALICE, gaseous detectors, eco-friendly gas mixtures.

Introduction

ALICE (A Large Ion Collider Experiment [1]) is one of the largest experiments hosted at CERN. The detector is mainly designed to study ultra-relativistic heavy-ion collisions in order to investigate the physics of strongly interacting matter at extreme energy densities, where the Quark Gluon Plasma (QGP) formation is expected [2]. The ALICE apparatus mainly includes high resolution tracking elements (ITS and TPC), particle identification detectors (TRD, TOF and HMPID), and the Forward Muon Spectrometer (FMS), including single-gap RPCs, for triggering purposes [3]. The resistive electrodes of the ALICE RPCs are made of 2 mm thick bakelite foils ($\rho \sim 10^{10} \Omega \text{ cm}$), separated by a 2 mm thick gas gap. These detectors operate in avalanche mode with a gas mixture made by tetrafluoroethane ($C_2H_2F_4 = 89.7\%$), isobutane ($i-C_4H_{10} = 10\%$), and sulfur hexafluoride ($SF_6 = 0.3\%$), discrimination threshold: 7 mV. The read-out planes are segmented in copper strips, connected to the front-end electronics (FEE). In particular all data presented in this work have been obtained through the new FEERIC (Front-End Electronics Rapid Integrated Circuit [4]) boards. The gas mixture used in the RPCs of the ALICE Muon Trigger (from now called simply ALICE mixture) has a negative environmental impact because of the presence of greenhouse gases (GHGs), ranked through their Global Warming Potentials (GWPs)¹. $C_2H_2F_4$, $i-C_4H_{10}$ and SF_6 have GWPs equal to 1300, 3 and 23500, respectively [5], leading to a total GWP for the ALICE

mixture of 1237. Beside the environmental problems, there is also an economic issue to consider. The EU planned a rapid reduction of GHG emissions through the Regulation (EU) N° 517/2014 [6]. In particular, the placing on market of fluorinated GHGs (included $C_2H_2F_4$ and SF_6) has been strictly reduced or even forbidden. As a consequence, there is a substantial price increase of the gases involved, which will continue over the years. For the reasons listed above, the goal of reducing GHG emissions has been set for the LHC experiments, as ALICE. Therefore, the aim of this work is to find a reasonable substitute for the ALICE mixture, in terms of efficiency, streamer probability², and operating voltage, but with a lower GWP.

Eco-friendly Gas Mixture

Since the main contribution to the GWP of the ALICE mixture is given by the percentage (89.7%) of $C_2H_2F_4$ (industrial name R134a), this study is focused on its replacement. The most promising alternative is the tetrafluoropropene $C_3H_2F_4$ with the trade name HFO1234ze [7] (for simplicity HFOze below). It has a chemical structure quite similar to R134a and a short atmospheric lifetime, bringing to a GWP lower than 10. A direct replacement of R134a with HFOze would not be advised because it would involve a considerable increase of the working point. Therefore, it is necessary to dilute it with another gas, such as CO_2 , in order to obtain HFOze-based mixtures with a lower operating voltage. Among the dif-

¹The GWP is the measure of how much heat a greenhouse gas traps in the atmosphere, relative to CO_2 whose GWP is 1.

²The streamer probability is an efficiency curve too, but obtained with a higher signal threshold.

ferent mixtures tested, the results for 11 mixtures will be reported. The components are always CO_2 , $HFOze$, $i-C_4H_{10}$ and SF_6 , but with different percentages. They are listed in table 1 (the ALICE mixture has been also collected but it is not included in the table). Since all the gas mixtures are made up of four different gases, the plan followed in order to study their properties has been to vary the concentrations of two components, keeping the amount of the other two gases constant. The tests performed may be divided in two phases:

1. **Tests on $HFOze/SF_6$ and $CO_2/HFOze$:** in order to evaluate the RPC efficiency in $HFOze$ -based mixtures with the addition of CO_2 and how the working point (HV_{eff}) and the streamer fraction³ are affected by the $HFOze$ and SF_6 variations.
2. **Tests on $i-C_4H_{10}/HFOze$ and $i-C_4H_{10}/CO_2$:** in order to probe the quenching properties of $i-C_4H_{10}$ in the new gas mixtures.

Mixture	CO_2	$HFOze$	$i-C_4H_{10}$	SF_6
M1	44.5	45.2	10.0	0.3
M2	44.5	44.5	10.0	1.0
M3	50.0	39.0	10.0	1.0
M4	50.0	39.7	10.0	0.3
M5	50.0	29.0	20.0	1.0
M6	50.0	34.0	15.0	1.0
M7	55.5	33.5	10.0	1.0
M8	60.5	33.5	5.0	1.0
M9	65.5	33.5	0.0	1.0
M10	59.0	35.7	5.0	0.3
M11	53.5	41.2	5.0	0.3

Table 1: Composition of the gas mixtures.

Experimental Set-up and Data Analysis

Data have been obtained by testing the gas mixtures with cosmic rays at the technological laboratories of the Istituto Nazionale di Fisica Nucleare (INFN) in Torino, during my master thesis work. It was used a small sized ALICE single-gap RPC ($50 \times 50 \text{ cm}^2$, 2 mm gas gap). The trigger was provided by the coincidence of three scintillators, coupled with photomultipliers, arranged above and below the detector. The high-voltage (HV) has been applied to the detector with temperature and pressure correction, given by the equation: $V_{app} = V_{eff} \frac{T_0 P}{T P_0}$ where $T_0 = 20^\circ C$ and $P_0 = 10^3 \text{ mbar}$. Before flushing the RPC, the mixture was bubbled in water at $10^\circ C$ ($\sim 40\%$ relative humidity), in order to preserve the resistivity of the bakelite electrodes. The threshold of the FEERIC boards was set at 70 mV after amplification (the choice of this threshold was based on tests performed on the ALICE RPCs at CERN). The analog signals from four strips in the trigger area were

³The RPCs of the ALICE FMS, as trigger detectors, have to be fast and selective. For this reason the streamer fraction at the operating voltage has to be as low as possible.

evaluated and stored through oscilloscope LeCroy WaveSurfer 510 (bandwidth = 1 GHz ; sampling rate = 10 GS/s) for the streamer analysis. All data are analysed offline through the Object-Oriented Data Analysis Framework ROOT. The parameters of interest are efficiency, working point, and streamer probability. All interpolations of the efficiency curves are performed with the following sigmoid function:

$$f(HV) = \frac{p_0}{1 + e^{-p_1(HV - p_2)}} \quad (1)$$

where p_0 is the maximum value of the curve, p_1 represents the steepness and p_2 is the HV value of the sigmoid midpoint. The errors on the efficiency are evaluated through the binomial statistic:

$$\sigma_\epsilon = \sqrt{\frac{\epsilon(1 - \epsilon)}{N_{trigger}}} \quad (2)$$

where ϵ is the efficiency value and $N_{trigger}$ is the number of events that have been triggered.

Tests and Results

Since the goal is to find a mixture with operating properties as close as possible to the ALICE mixture, before starting studies on RPC performances with the new gas mixtures, the detector has been characterized with the ALICE one. In figure 1 is reported the obtained efficiency curve which represents the “benchmark” to refer to.

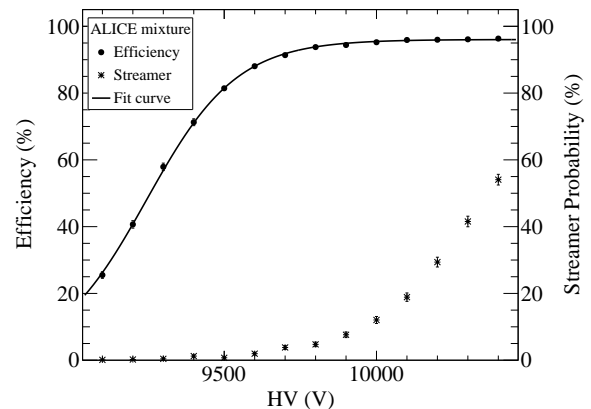


Figure 1: Efficiency curve and streamer probability of the RPC detector equipped with FEERIC boards, fluxed with the ALICE mixture, and measured with cosmic rays.

The study started by varying the ratio between $HFOze$ and SF_6 , in order to evaluate the role of SF_6 as a streamer suppressor in $HFOze$ -based mixtures. The percentages of CO_2 and $i-C_4H_{10}$ are kept constant. In figure 2.a is shown the comparison between mixtures M1 and M2 of table 1.

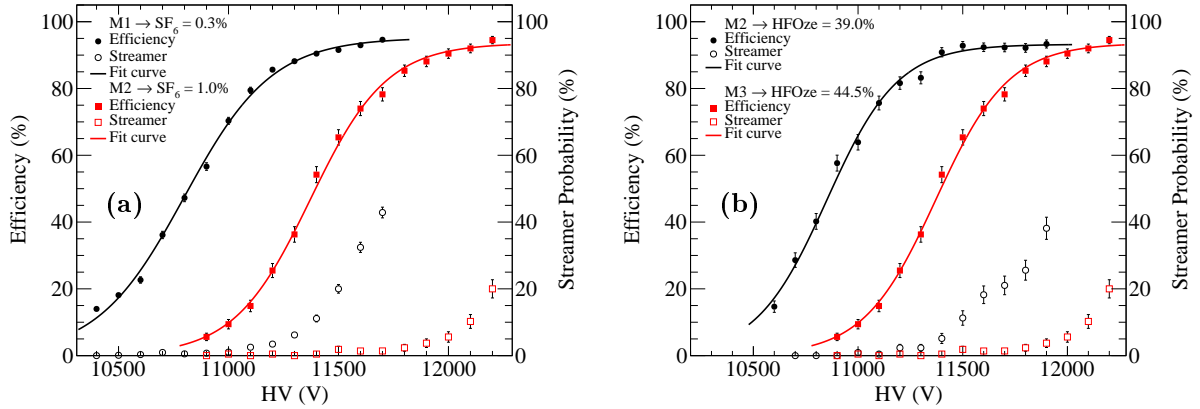


Figure 2: Efficiency and streamer probability for HFOze-based mixtures with different HFOze/SF₆ concentration (mixtures 1 and 2 of table 1) (a) and HFOze/CO₂ concentration (mixtures 2 and 3 of table 1) (b).

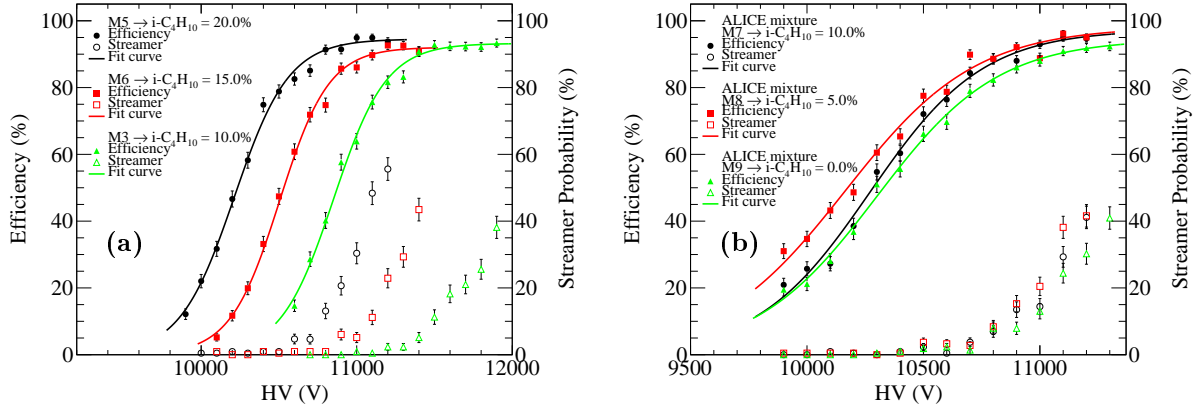


Figure 3: *i*-C₄H₁₀ effects on streamer suppression. *i*-C₄H₁₀/HFOze variation passing from 20.0% to 10.0% (mixtures 5, 6, and 3 of table 1) (a) and *i*-C₄H₁₀/CO₂ variation passing from 10.0% to 0.0% (mixtures 7, 8, and 9 of table 1) (b).

The streamer probability for the mixture with 1.0% SF₆ is much lower than the one with 0.3% SF₆. The SF₆ effect is to increase the separation between the efficiency and the streamer curves, resulting in a lower streamer probability at the working point. In addition a small variation of SF₆ leads to a considerable increase of the operating voltage (~ 500 V from 0.3% to 1.0% SF₆). Instead, in figure 2.b is shown a decrease of CO₂ with an increase of HFOze, while *i*-C₄H₁₀ and SF₆ concentrations are kept constant. The plot consists in the comparison of the mixtures M2 and M3 reported in table 1. Data suggest the presence of a linear correlation between the variation of HV_{eff} and the HFOze percentage, that may be quantified. In particular an increase of ~ 5% HFOze leads to an increase of the working point of about 500 V. In addition the streamer probability of the mixture with 44.5% HFOze seems to be slightly lower than the one with 39.0% HFOze. This (as well as the increase of the working point) is probably due to HFOze electronegativity properties, which help to confine the signal size, by absorbing electrons. Moreover, the effects on HV_{eff} due to HFOze and SF₆ are indepen-

dent. This may be observed by comparing mixture M1 with M3 and mixture M2 with M4 of table 1 (for more information about these plots, the reader is referred to the master thesis work [8]). In the first case the mixture M1 has about +5% of HFOze but -0.7% of SF₆ with respect to the mixture M3, leading to a null net result on HV_{eff} shift and to overlapped curves. In the second case the mixture M2 has ~ 5% HFOze and 0.7% SF₆ more than mixture M4. As a consequence the separation between the two efficiency curves is of ~ 1000 V. In both comparisons there is a lower streamer probability for the mixture with more SF₆, as expected. As next step the effects on the streamer probability were analyzed by varying the concentrations of *i*-C₄H₁₀/HFOze (mixtures 5, 6 and 3 of table 1) and of *i*-C₄H₁₀/CO₂ (mixtures 7, 8 and 9 of table 1). In particular, *i*-C₄H₁₀ concentration has been gradually reduced, with steps of 5%. The percentage taken from *i*-C₄H₁₀ has been added first to HFOze (going from 20.0% to 10.0% of *i*-C₄H₁₀), and then to CO₂ (going from 10.0% to 0.0% of *i*-C₄H₁₀). Results are shown in figure 3. In figure 3.a the percentages of *i*-C₄H₁₀ and

HFOze are varied by keeping constant the CO_2 and SF_6 ones. The shift of the working point is due to the increase of HFOze. The streamer probability progressively decreases with $i-C_4H_{10}$ reduction and therefore, with the increasing of HFOze. In figure 3.b the percentages of $i-C_4H_{10}$ and CO_2 are varied by keeping constant HFOze and SF_6 ones. The efficiency curves are quite clustered and there not seems to be a significant contribution on streamer probability due to $i-C_4H_{10}$ variation.

ALICE mixture Comparison and Conclusions

Among all the mixtures tested, the best results in terms of efficiency, streamer probability, working point, and GWP have been obtained with the mixtures 4, 10, and 11 of table 1. In figure 4 and in table 2 is shown a comparison with the ALICE mixture: the most promising HFOze-based mixtures show an increase of the operating voltage of $\sim 1000 V$ and a higher streamer probability, with a good efficiency and a considerable reduction of the GWP (~ 17 times lower). Several interesting features have been emerged by testing gas mixtures made up of HFOze, CO_2 , $i-C_4H_{10}$ and SF_6 .

A linear relation among the variations of HFOze and SF_6 , and the shift of the detector working point has been found. In particular a variation of $\sim 5\%$ HFOze or $\sim 0.7\%$ SF_6 leads to a shift of $\sim 500 V$ in both cases. Moreover $i-C_4H_{10}$ effects on streamer suppression in HFOze-based mixtures are not noticeable because those of HFOze and SF_6 are predominant. Concerning R134a replacement with HFOze and CO_2 , promising results have been obtained, even though lower operating voltage and streamer probability would be advisable.

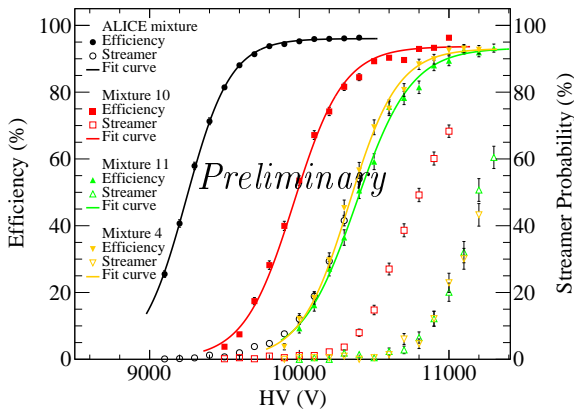


Figure 4: Comparison among the ALICE mixture and the most promising HFOze-based mixtures.

Mixture	HV_{eff} (V)	Eff. (%)	Stream. (%)	GWP
ALICE	9900	94.4 ± 0.5	7.8 ± 0.9	1237
M4	11000	93 ± 1	23 ± 3	73
M10	10800	92.9 ± 0.7	49 ± 2	73
M11	11100	93 ± 1	32 ± 3	73

Table 2: Summary of the efficiency (Eff.) and the streamer probability (Stream.) at the operating voltages (HV_{eff}) of the ALICE mixture and the most promising HFOze-based mixtures, found so far. Their GWPs are also shown.

References

- [1] AAMODT, K. ET AL.: *The ALICE experiment at the CERN LHC*. Journal of Instrumentation 3.08, S08002, (2008).
- [2] BAZAVOV, A. ET AL.: *Chiral and deconfinement aspects of the qcd transition*. Physical Review D 85, 054503, (2012).
- [3] FABJAN, C., SCHUKRAFT, J.: *The story of ALICE: Building the dedicated heavy ion detector at LHC*. arXiv:1101.1257, (2011).
- [4] DUPIEUX, P. ET AL.: *Upgrade of the ALICE Muon Trigger electronics*. Journal of Instrumentation 9.09, C09013, (2014).
- [5] MYHRE, G. ET AL.: *Anthropogenic and Natural Radiative Forcing*. In: *Climate Change 2013: The Physical Science Basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change* [Stocker, T.F. et al. Report of the Intergovernmental Panel on Climate Change. Cambridge University Press, Cambridge, United Kingdom and New York, NY, USA, (2013).
- [6] THE EUROPEAN PARLIAMENT AND THE COUNCIL OF THE EUROPEAN UNION: *Regulation (EU) N° 517/2014 of the European Parliament and of the Council of 16 April 2014 on fluorinated greenhouse gases and repealing Regulation*. Official Journal of the European Union, L 150/196, (2014).
- [7] HONEYWELL: *Solstice ze Refrigerant (HFO-1234ze (E)). The Environmental Alternative to Traditional Refrigerants. Ultra-low GWP Hydrofluoroolefins (HFO)*. www.honeywell-refrigerants.com.
- [8] ROSANO, A.: *Studies on eco-friendly gas mixtures for the Resistive Plate Chambers of the ALICE Muon Identifier*. Master's thesis, Università degli Studi di Torino, Turin, Italy (2019).

Effect of temperature on the absorption spectrum of Lithium deposited on argon cluster

A. Saidi^{1,*}

¹*Dipartimento di Scienze Matematiche e Informatiche, Scienze Fisiche e Scienze della Terra, Università degli Studi di Messina, viale F. Stagno d'Alcontres 31, Messina, Italy*

*Corresponding Author email: saidiagir83@gmail.com

Abstract

Photoabsorption spectra of LiAr_n ($n = 2 - 3$) are simulated at temperatures ranging between 5 and 16 K. The calculations associate a Monte Carlo (MC) method to sample cluster geometries at temperature T , with a one electron ab initio model to calculate the ground-state and excited-state energies of the cluster. The latter model replaces the Li^+ core electrons and all the electrons of the Ar atoms by appropriate pseudopotentials, complemented by core polarization potentials. It also provides the necessary oscillator strengths to simulate the spectra. Global optimization by basin-hopping is used in combination with MC simulation at low temperature (5 K) to identify the most stable isomer and remarkable isomers of ground-state LiAr_n clusters, which are stable with respect to deformations of the order of those expected with Zero Point Energy motions. The absorption spectra calculated for each of these isomers at 5 K suggest that absorption spectroscopy can probe sensitively the local (number of Ar atom in close vicinity, and local symmetry about Li. Simulation at increasing temperatures, up to the evaporation limit of Li out of the cluster, shows the onset of large amplitude motions above 20 K, when the Li atom experiences a variety of local environments.

Keywords: .

Introduction

The electronically excited states of a chromophore bonded to rare-gas atoms are very sensitive to the interaction between the chromophore and its environment. This has motivated numerous experimental and theoretical works for two reasons, essentially. One was to explore microsolvation by rare-gas atoms. For instance, the microsolvation of aromatic molecules was pioneered in the group of Leutwyler [1] and further developed elsewhere [2-4]. The second motivation appeared in theoretical works, where the chromophore spectroscopy is proposed as a sensitive probe of the structure and phase (liquid or solid) of the rare-gas moiety that interacts with the chromophore. This point of view appeared in a series of works where the chromophore is a single alkali [5-7], alkaline earth [8,9], or boron [10] atom. The Photoabsorption spectrum of Ca in CaAr_n cluster was also proposed as a way to prove the relaxation dynamics of these clusters when placed out of equilibrium [11].

Theoretical

The absorption spectra are simulated in three steps. First, an MC random walk is used to select a series of geometries that are representative of ground-state LiAr_n clusters at temperature T . The random walk is initiated from the absolute minimum of the ground-state potential

energy surface (the procedure used to find this geometry will be described in a later section). The global minimum of the LiAr_n ($n = 2, 3$) clusters as several remarkable isomers of higher energy are also presented in the present work. The cluster energies required by the MC algorithm are provided by the one-electron ab initio model. The same model is used in the second step to provide electronic energies and oscillator strengths for exciting the KAr_n clusters from the ground state. This calculation is performed for each cluster geometry selected in the first step. A histogram of the transition intensities (deduced from the oscillator strengths) is built in the third step as a function of the excitation energy. It simulates the absorption spectrum according to the vertical transition approximation. This approach is semi classical since the transition energies and strengths are obtained quantum mechanically and the geometries, classically.

The One-Electron ab Initio Model:

The one-electron model is fully described in ref [12]. Shortly, works in the late 1960s showed that the interaction in alkali-rare gas pairs is governed primarily by the unique valence electron of the alkali atom and can be described accurately using ultra large core pseudopotentials complemented by core-polarization potentials, which substitute all the electrons of the rare-gas atom and all those of the alkali ion core [24-27] This approach was generalized in the 1990s and later to describe al-

kali atoms interacting with several (or many) rare-gas atoms [6,13-16]. The pseudopotentials used here are of the l -dependent semilocal type, according to the expression of Barthelat and Durand [31] and F. Spiegelman [17]. The single valence electron pseudopotential for the $[K+]$ core has been widely used in accurate standard valence calculations [18]. Argon was treated as a zero-electron atom with all its electrons in the core via an atomic $[Ar]$ core pseudopotential determined by Duplaa and Spiegelman [17]. The pseudopotentials also incorporate core polarization operators (so-called core-polarization potentials) using the l -dependent formulation of Foucault and co-workers [19] generalizing the initial formulation proposed by Muller and Meyer [20]. This method solves the electronic problem, whereas the full Hamiltonian includes the core-core interactions.

Sampling Geometries in Ground-State Potential Energy Surfaces:

The geometry sampling is performed using an MC random walk within the ground-state potential energy surface of the $LiAr_n$ clusters. The starting geometry is the global minimum of this surface (40 (see next section)). The random walk exploration is performed by choosing an atom (Li or any Ar atom) randomly and displacing it by a maximal distance from $0.25 a_0$ to $1.0 a_0$, depending on the acceptance yield, along one of the axes x , y , or z , also chosen randomly. The atoms are confined inside a sphere of $50 a_0$ radius, but the calculation was stopped when an atom evaporates from the considered cluster. The energies of the ground- and of the i th excited- state E_i^k of the KAr_n cluster at the k th MC iteration are provided by the one-electron *ab initio* calculation (see previous section). The new configuration ($k + 1$) is accepted or rejected according to the Metropolis criterion [21] applied to the state of interest: always accepted when $E_i^{k+1} < E_i^k$ and when $E_i^{k+1} > E_i^k$, according to the $\exp\left(\frac{-(E_0^{k+1} - E_0^k)}{k_b T}\right)$ probability. The number of MC steps used for the calculations was limited to 20000 by atoms of the clusters. This methodology provides an MC trajectory within the configuration space of the KAr_n clusters. It corresponds to a series of cluster geometries, labelled R_k , that are representative of those populated at temperature T .

Determination of Structures:

Structures are identified using the basin-hopping technique [42]. Their stability with respect to Zero Point Energy (ZPE) motions was checked qualitatively by running an MC simulation at 5 K. The latter temperature was chosen to be close to the expected ZPE. Of course, since the atoms are considered classically in the present work, we do not claim ZPE motions are taken into account quantitatively. The objective here is to check that the structures that were identified are stable with respect to motions that are of the same order of magnitude as the expected ZPE. Furthermore, at this temperature it was demonstrated that the ZPE effect on the properties

of the cluster was negligible [9]. Ar_n clusters were also shortly investigated using the interaction potential previously presented. MC trajectory was calculated at $T = 20$ K, followed by a freezing at 1 K for identified structures. The optimal structures found fit perfectly the one of the Cambridge Cluster Database [23], using the same potential. The present calculation provides also isomers and the corresponding energies, which will be used in the following discussion.

Simulation of the Absorption Spectrum:

At each geometry R_k , electronic energies $E_m(R_k)$ and transition dipole moments $D_{0m}(R_k)$ are calculated using the one-electron model. A histogram is built from integration of the transition energies $E_{0i} = E_i(R_k) - E_0(R_k)$ and the transition intensities along the MC trajectory.

Results and Discussion

Low-Energy Isomers of Ground-State $LiAr_n$ Clusters:

The optimized equilibrium geometries of the systems are shown in Figures 1, 2 respectively. We note that in the case of the neutral in the $2s$ state, the lithium atom remains weakly attached and only slightly disturbs the geometry of the argon structure which forms a small. This is because the Li-Ar interaction energy (42 cm^{-1}) [23] is weaker than the Ar-Ar interaction energy (99 cm^{-1}). The geometry of the argon part is almost the same as that of the pure argon cluster and this because of the repulsion of the electron of state $2s$ with the atoms of argon and the orbital $2s$ is only slightly disturbed by the cluster. The equilibrium geometry of neutral aggregates $LiAr_n$ is the geometry of higher symmetry. In the case of $n = 2$, the triangle is isosceles formed by an atom of Lithium and the two atoms of argon with $R_{ArAr'} = 7.09 a_0$, close to the equilibrium distance Ar-Ar of the potential of LJ used in our work ($r_m = 7.10 a_0$). This last value is comparable with the distance Ar-Ar found experimentally in Ar_2 ($7.18 a_0$) [24]. For $n = 3$, the structure of $LiAr_3$ has a C_{3v} symmetry in a trigonal pyramid. We call this structure "substituted" since the lithium atom appears as a substitute in Ar_{n+1} structures reported by Wales and Doyes [25].

Simulation of the absorption spectrum:

The objective is to illustrate the sensitivity of the absorption spectra to the local environment of Lithium. The simulations are carried out at the same temperature $T = 5$ K for the $LiAr_2$ aggregate and the $LiAr_3$ cluster, a temperature which preserves the metastability of the isomers.

We observe that the absorption spectra reflect a degeneration of the Li ($2p^2 P$) state by the argon atoms which surround the Lithium. Two types of bands appear in the two figures. A band, single or double depending on the value of n of $LiAr_n$, is moved in the red compared

to the atomic transition. It corresponds to a molecular level twice degenerate for $n = 2$ whose degeneration is lifted for $n = 3$. We call it band π with reference to a "pseudo-diatomic" description of the interaction Li (remember that Li is found on the surface of the argon cluster figure 1). The other band is moved in the blue of the atomic transition, it is called band Σ . We thus find the degeneration 3 of the p_x, p_y, p_z orbitals of an isolated atom in the case of LiAr_2 . The π band is therefore stabilizing (the excited atom cannot detach itself from the aggregate by its electronic energy), the second is destabilizing (the system has the energy to be able to eject the metal atom).

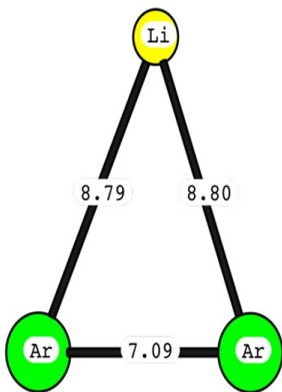


Figure 1: Optimized structure of LiAr_2

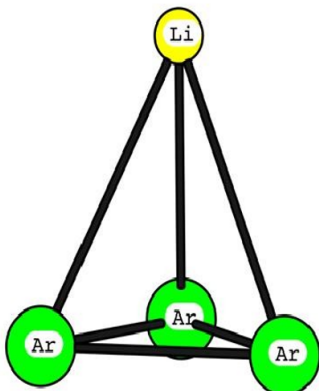


Figure 2: Optimized structure of LiAr_3

To facilitate the discussion on the spectra of figure 3 and figure 4, we have drawn on figure 5 the orbital contour of the three excited states of the aggregate $\text{Li}(2p)\text{Ar}_{2,3}$. Thus, we observe that the states of Atomic Lithium can undergo a degeneration lift according to the orientation of the orbitals with respect to the argon atoms of the

cluster. The first reason is symmetry, if we take into account that the first argon neighbors: in the spectrum of the aggregate LiAr_2 , we have a C_{2v} symmetry, the two components $2p_x$ and $2p_y$ are not identically deformed, because they don't see the same first neighbors the same way. On the other hand, in the spectrum of the LiAr_3 cluster has a C_{3v} symmetry, the two components $2p_x$ and $2p_y$ of the $2p$ orbital are parallel to the argon plane. They are then deformed in the same way by the immediate argon neighbours (see figure 5), hence the degeneration of the line π figure 4.

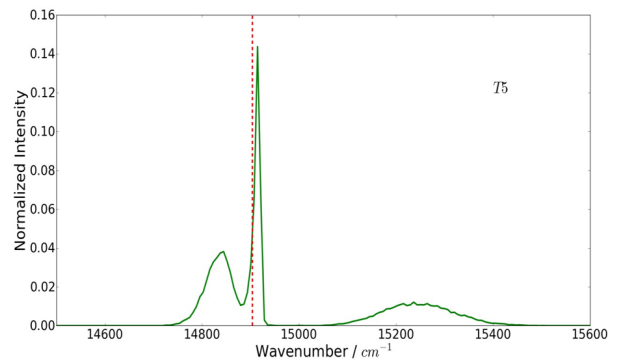


Figure 3: LiAr_2 absorption spectrum at $T = 5\text{ K}$ from the ground state to the excited state $2p$. Dotted in red the line of the isolated Lithium atom, calculated without spin-orbit interaction.

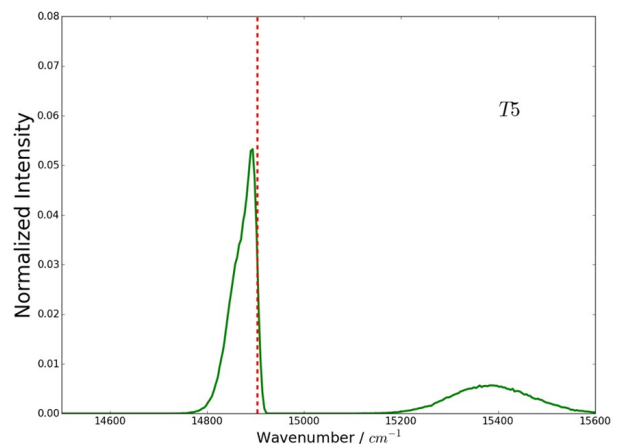


Figure 4: LiAr_3 absorption spectrum at $T = 5\text{ K}$ from the ground state to the excited state $2p$. Dotted in red the line of the isolated Lithium atom, calculated without spin-orbit interaction.

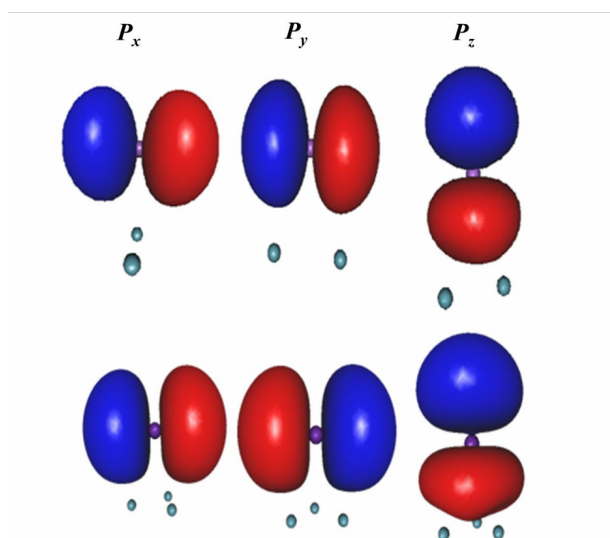


Figure 5: The p_x , p_y , p_z orbitals of the stable configuration of LiAr_2 and LiAr_3 .

Absorption spectrum: Effect of temperature:

In this part, we will briefly present the results of the numerical simulations carried out by the dynamic process based on the Metropolis algorithm. Let us add that in the results presented, we maintained the system in a sphere of radius 27 Å to maintain its cohesion. This method allowed us to obtain the absorption spectra of the aggregates of size $n = 2$ and $n = 3$. We have seen that the general shape of the spectrum is not modified by the change in the number of accepted configurations, which shows that our calculation reaches thermalization.

Temperature effect of the absorption spectrum of LiAr_2 :

Figure 6 shows the absorption spectra from the fundamental state $2s$ to the first excited state $2p$: $\text{Li} (2s \rightarrow 2p) \text{Ar}_2$ simulated at various temperatures by the Monte Carlo method. Each spectrum is obtained for approximately 7.5×10^4 steps MC. We observed from $T = 16$ K the evaporation of the Li atom. The two sub-bands Π and the band Σ are clearly identical in the spectrum for $T = 6$ K to that for $T = 5$ K: ne are not affected in the same way when the temperature rises. Indeed, the band becomes wider and moves towards the atomic transition of Li (line dotted in red: $\nu = 14908 \text{ cm}^{-1}$) while the sub-bands merge into a single broad band, with a very high peak close to the atomic transition of Li. Its observations are consistent with spectra when temperatures are high, breaking the C_{2v} symmetry of the LiAr_2 aggregate and moving the atoms away from their equilibrium position.

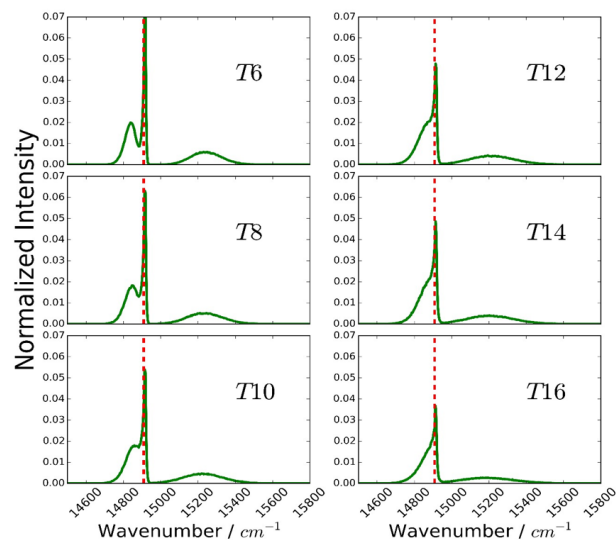


Figure 6: LiAr_2 absorption spectrum for temperatures ranging from $T = 6$ K to $T = 16$ K.

Conclusion

We have simulated the absorption spectrum of the LiAr_n cluster ($n = 2,3$) where a single lithium atom is linked to a small number of argon atoms. A Basin-Hopping type global optimization method in combination with a Monte-Carlo method in the ground state at a low temperature ($T = 5$ K) is used to find the most stable configurations and the low energy isomers of our aggregates. In the most stable isomers, the Li atom is on the surface of a compact structure formed by Argon atoms. The low temperature simulation makes it possible to check the stability or the metastability of these isomers with respect to the deformation of the order of those expected with ZPE movements. The absorption spectra calculated for each of these isomers at 5K suggests that absorption spectroscopy sensitively probes the local symmetry around the Li atom. The location on the surface of Li with respect to the aggregate appears as a division of $2s \rightarrow 2p$ into two components called band Σ and Π . The increase in temperature causes the fusion of two sub-bands into a single band displaced towards the atomic line of Li and a widening of the band, subsequently showing an evaporation of the atom of Li from a temperature of $T = 16$ K.

References

1. Leutwyler, S.; Boesiger, J. Rare-gas Microsolvation of Aromatic Molecules. *Z. Phys. Chem.* 1987, 154, 31.
2. Brechignac, P.; Coutant, B. Microsolvation of Aniline by Argon: Fluorescence Excitation and Two Photon Resonant Ionization of AnAr_n in a Supersonic Jet. *Z. Phys. D: At., Mol. Clusters* 1989, 14,

- 87-88.
- Perera, L.; Amar, F. G. Spectral Shifts and Structural Classes in Microsolutions of Rare Gas Clusters Containing a Molecular Chromophore. *J. Chem. Phys.* 1990, 93, 48844897.
 - Schmidt, M.; Mons, M.; Le Calve, J. Microsolvation of the Benzene Molecule by Argon Atoms: Spectroscopy and Isomers. *Chem. Phys. Lett.* 1991, 177, 371379.
 - Martyna, G.; Cheng, C.; Klein, M. L. Electronic States and Dynamical Behavior of LiXen and CsXen clusters. *J. Chem. Phys.* 1991, 95, 13181336.
 - Tsoo, C. C.; Estrin, D. A.; Singer, S. J. Electronic Spectra of NaAr₄ and NaAr₆ - Isomerization and melting. *J. Chem. Phys.* 1992, 96, 79777991.
 - Boatz, J. A.; Fajardo, M. E. Monte Carlo Simulations of the Structures and Optical Absorption Spectra of Na Atoms in Ar Clusters, Surfaces, and Solids. *J. Chem. Phys.* 1994, 101, 34723487.
 - Calvo, F.; Spiegelman, F.; Gaveau, M. A.; Briant, M.; Fournier, P. R.; Mestdagh, J. M.; Visticot, J. P. Spectroscopic Manifestations of Phase Changes in CaAr_n Clusters: Finite Size Effects. *Eur. Phys. J. D* 2003, 24, 215218.
 - Calvo, F.; Spiegelman, F.; Heitz, M.-C. Theoretical Study of Finite-Temperature Spectroscopy in Van der Waals Clusters. I. Probing Phase Changes in CaAr_n. *J. Chem. Phys.* 2003, 118, 8739 8753.
 - Krumrine, J. R.; Alexander, M. H.; Yang, X.; Dagdigian, P. J. Experimental and Theoretical Study of the Electronic Spectrum of the BaAr₂ Complex: Transition to the Excited Valence B(2s2p22D) state. *J. Chem. Phys.* 2000, 112, 50375043
 - Calvo, F.; Spiegelman, F.; Wales, D. J. Theoretical Study of Finite-Temperature Spectroscopy in Van der Waals Clusters. II. Time Dependent Absorption Spectra. *J. Chem. Phys.* 2003, 118, 87548762.
 - Rhouma, M. B. E. H.; Berriche, H.; Lakhdar, Z. B.; Spiegelman, F. One-Electron Pseudopotential Calculations of Electronic Properties of NaAr *n*: Low-Energy Isomers and Absorption Spectra. *Int. J. Quantum Chem.* 2004, 99, 495501.
 - Groß, M.; Spiegelmann, F. A Pseudopotential Study of Molecular Spectroscopy in Rare Gas Matrices: Absorption of NO in Argon. *Eur. Phys. J. D* 1998, 4, 219224.
 - Rhouma, M. B. E. H.; Ben Lakhdar, Z.; Berriche, H.; Spiegelman, F. Rydberg States of Small NaAr_n* Clusters. *J. Chem. Phys.* 2006, 125, 084315.
 - Douady, J.; Jacquet, E.; Giglio, E.; Zanuttini, D.; Gervais, B. Solvation of Na²⁺ in Ar_n clusters. I. Structures and Spectroscopic Properties. *J. Chem. Phys.* 2008, 129, 184303.
 - Jacquet, E.; Zanuttini, D.; Douady, J.; Giglio, E.; Gervais, B. Spectroscopic Properties of Alkali Atoms Embedded in Ar Matrix. *J. Chem. Phys.* 2011, 135, 174503.
 - Duplaa, P.; Spiegelmann, F. A Pseudopotential Hole-Particle Treatment of Neutral Rare Gas Excimer Systems 0.2. The Rydberg States of the Ar₂* Dimer. *J. Chem. Phys.* 1996, 105, 15001515.
 - Rhouma, M. B. E.; Berriche, H.; Lakhdar, Z. B.; Spiegelman, F. One-Electron Pseudopotential Calculations of Excited States of LiAr, NaAr, and KAr. *J. Chem. Phys.* 2002, 116, 18391849.
 - Foucrault, M.; Millie, P.; Daudey, J. P. Non Perturbative Method for Core Valence Correlation in Pseudopotential Calculations-Application to Rb₂ and Cs₂ molecules. *J. Chem. Phys.* 1992, 96, 12571264.
 - Muller, W.; Flesch, J.; Meyer, W. Treatment of Intershell Correlation Effects in ab initio Calculations by Use of Core Polarization Potentials. Method and Application to Alkali and Alkaline Earth Atoms. *J. Chem. Phys.* 1984, 80, 32973310.
 - Metropolis, N.; Rosenbluth, A. W.; Rosenbluth, M. N.; Teller, A. H.; Teller, E. Equation of State Calculations by Fast Computing Machines. *J. Chem. Phys.* 1953, 21, 10871092.
 - Wales, D. J.; Doye, J. P. K.; Dullweber, A.; Hodges, M. P.; Naumkin, F. Y.; Calvo, F.; Hernandez-Rojas, J.; Middleton, T. F. The Cambridge Cluster Database. URL <http://www-wales.ch.cam.ac.uk/CCD.html>, 2006.
 - Bokelmann, F., & Zimmermann, D. (1996). Determination of the K-Ar interaction potential in the X and A state from laser spectroscopic data. *The Journal of chemical physics*, 104(3), 923-934.
 - Ulrich, B.; Vredenburg, A.; Malakzadeh, A.; Schmidt, L. P. H.; Havermeier, T.; Meckel, M.; Cole, K.; Smolarski, M.; Chang, Z.; Jahnke, T.; et al. Imaging of the Structure of the Argon and Neon Dimer, Trimer, and Tetramer. *J. Phys. Chem. A* 2011, 115, 69366941.
 - Wales, D. J.; Doye, J. P. K.; Dullweber, A.; Hodges, M. P.; Naumkin, F. Y.; Calvo, F.; Hernandez-Rojas, J.; Middleton, T. F. The Cambridge Cluster Database., 2006.

**SEMINARI
DEL DOTTORATO DI RICERCA
IN FISICA
(Svolti nel 2019)**

SEMINARI DEL DOTTORATO DI RICERCA IN FISICA

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

18 Gennaio 2019, ore 10.00, Sala seminari, CNR-IPCF
V.le F. Stagno d'Alcontres 37, S. Agata, Messina

Matter and devices: beyond silicon, what next?

Dott. Rosario Corrado Spinella
Direttore del Dipartimento di Scienze Fisiche e Tecnologie della Materia del CNR

Abstract

We are experiencing an impressive improvement of microscopy techniques with achievable resolution having approached a level that makes possible to probe individual atoms. This progress has been driven by the effort to achieve a better understanding of the physical properties of materials and devices whose feature sizes are in the range of the nanometer scale. The talk will address the importance of these techniques in characterizing novel materials of interest for the future trend in microelectronics.

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

7 Febbraio 2019, ore 15.00, Incubatore d'Impresa Aula HT10/11-T
V.le F. Stagno d'Alcontres 31, 98166 S. Agata, Messina

L'Esplorazione Spaziale del Sistema Solare: un Viaggio alla Scoperta dei Pianeti

Dott. Giuseppe Sindoni
ASI - Agenzia Spaziale Italiana

Abstract

Sin dagli albori della civiltà l'uomo è stato spinto verso l'esplorazione di luoghi sconosciuti. Negli anni '50, con l'avvento della tecnologia spaziale tale impulso si è spinto oltre il nostro pianeta. Da allora e fino ad oggi sono stati esplorati molti corpi extraterrestri del nostro sistema solare mediante l'impiego di sonde spaziali. L'Italia è sempre stata in prima fila nello sviluppo di tecnologia all'avanguardia e nell'analisi dei dati provenienti da missioni spaziali di grande impatto per l'esplorazione planetaria. In particolare, l'Agenzia Spaziale Italiana (ASI), in collaborazione con gli enti di ricerca, tra i quali INAF e CNR, e le università, ha partecipato attivamente a decine di missioni spaziali, sia NASA che ESA, con grandissimo successo. Basti pensare per esempio a MarsExpress (MEX) ed ExoMars su Marte, Juno su Giove e Cassini su Saturno. Anche il futuro riserverà grandi sorprese con la partecipazione italiana alle missioni BepiColombo su Mercurio, JUICE su Giove e CHEOPS, PLATO e ARIEL per la caratterizzazione dei sistemi esoplanetari. Le informazioni che si possono ottenere dalla strumentazione montata a bordo delle sonde spaziali sono molteplici: dalla composizione della superficie dei pianeti rocciosi e dei satelliti naturali alla caratterizzazione delle atmosfere ed esosfere planetarie così come della loro climatologia. Inoltre, i dati e le immagini straordinarie che ci arrivano quotidianamente dallo spazio ci aiutano a monitorare l'evoluzione di particolari fenomeni chimico/fisici utili per la comprensione del nostro sistema Terra. In questa presentazione forniremo una panoramica sulle missioni spaziali con coinvolgimento diretto dell'Italia e sui relativi risultati scientifici che hanno profondamente migliorato la comprensione del nostro sistema solare.



DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

21 Febbraio, ore 15.00, Incubatore d'Impresa Aula HT10/11-T
V.le F. Stagno d'Alcontres 31, 98166 S. Agata, Messina

The Extreme Energy Events Project

Dr.ssa Paola La Rocca

*Dipartimento di Fisica e Astronomia, Università di Catania, INFN -sez. di Catania, Museo Storico della Fisica e
Centro Studi e Ricerche "Enrico Fermi"*

Abstract

The Extreme Energy Events Project is an experiment aimed at the detection of secondary cosmic ray muons. It consists of a sparse array of about 50 telescopes distributed throughout the Italian territory, covering an area of $3 \times 10^5 \text{ km}^2$. Its distinctive feature is that the telescopes, based on Multigap Resistive Plate Chambers (MRPC), are housed in High Schools and managed by groups of students and teachers. About 100 billion muon tracks have been stored and analyzed since the first coordinated data taking in 2014. The analysis activity is currently in progress and focused on several items: coincidence searches of muons from the same EAS and long distance correlations between different EAS, study of time variations of the muon flux on ground level, searches for large scale cosmic ray anisotropy and for upward-going particles. In this presentation an overall description of the experiment will be given, together with its educational fallout. The operation of the whole array is also presented by showing the most recent results obtained from the analysis of the collected data.

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

21 Marzo 2019, ore 15:00, Incubatore d'Impresa Aula HT10/11-T
V.le F. Stagno d'Alcontres 31, 98166 S. Agata, Messina

Il metodo scientifico attraverso le opere di Archimede, Galilei e Majorana

Dott. Angelo Pagano
INFN, sezione di Catania

Abstract

Nel corso del seminario saranno tracciati i tratti essenziali del metodo scientifico attraverso l'esame di (necessariamente) brevi riferimenti ai lavori di Archimede, Galileo Galilei ed Ettore Majorana. Il tratto caratteristico dei tre grandi scienziati risulta nel rigore logico-matematico adottato nella descrizione dei fenomeni naturali, siano essi di carattere macroscopico che microscopico, e nella coerenza al metodo scientifico che, da Galileo in poi, si suole definire sperimentale.

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

28 Marzo 2019, ore 9.30, Camera di Commercio

Piazza F. Cavallotti, 3 - 98122 Messina

Career Day, per la prima volta a Messina, l'evento AlmaLaurea per chi cerca lavoro

Abstract

Laureandi e laureati di Sicilia e Calabria si ritrovano quest'anno a Messina per incontrare decine tra le più importanti aziende nazionali ed internazionali alla ricerca di giovani talenti. L'edizione 2019 di "Al Lavoro", il Career Day più atteso dell'anno in cui i più importanti responsabili delle risorse umane incontrano laureandi e laureati, è promosso dal COP Unime e organizzato da AlmaLaurea, il consorzio interuniversitario fondato nel 1994 a cui ad oggi aderiscono 75 Atenei. L'appuntamento è per giovedì 28 marzo, presso la Camera di Commercio di Messina (Piazza Cavallotti, 3), chi volesse partecipare può già aggiornare il proprio CV AlmaLaurea (chi non lo avesse può crearlo adesso qui), registrarsi al career day e selezionare le imprese a cui segnalare la propria candidatura per un colloquio one-to-one. È possibile partecipare alla giornata anche senza registrare il proprio colloquio per incontrare i recruiter di tutte le imprese partecipanti, scoprire quali sono le posizioni aperte e consegnare il proprio CV, nonché incontrare gli enti di formazione presenti. Tra le aziende che saranno presenti si segnalano Alleanza Assicurazioni, Alten Italia, Automazioni Industriali Capitano, Blue Reply, Capgemini Italia, Carrefour, Consoft Informatica, Costa Crociere, Indra - Minsait, Italdesign, KPMG, Leroy Merlin, Lidl Italia, Ntt Data Italia, Previnet, QiBit, Sonatrach Raffineria Italiana, Schneider Electric, Spindox, TXT E-Solutions, Volotea ed Eurobindo. Un'occasione unica per i laureandi e i neo-laureati per affacciarsi al mondo del lavoro. Per ulteriori informazioni o assistenza è possibile consultare le F.A.Q. o scrivere a supporto.laureati@almalaurea.it.

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

9 Aprile 2019, ore 15.00, Sala seminari, CNR-IPCF

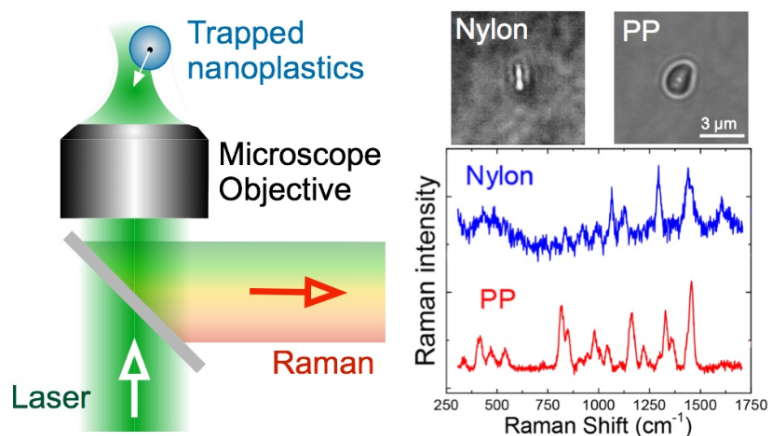
V.le F. Stagno d'Alcontres 37, S. Agata, Messina

Plasmonics for molecular detection and Raman tweezers coupled with thermo-plasmonics for micro- and nano-plastics detection

Prof. Raymond Gillibert
CNR-IPCF, Messina

Abstract

In a first part the near-field and far-field plasmonic properties of a new family of hybrid substrates designed to combine surface plasmon resonance imaging (SPRi) and Surface Enhanced Raman Scattering (SERS) consisting of gold nanoparticles deposited on a gold film will be presented. Pico-molar SERS sensing will be demonstrated using an aptamer. Raman tweezers will be proposed as a new analytical method for nano and microplastics detection. Nano-plastic detection and identification will be demonstrated in sea water as well as differentiation from naturally occurring sediments. Thermoplasmonic-enhanced trapping will then be used to improve the particle detection using nano structured surfaces.



DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

14 Maggio 2019, ore 9.30, Sala seminari, CNR-IPCF
V.le F. Stagno d'Alcontres 37, S. Agata, Messina

Appunti di Fisica Teorica 10

Dott.ssa Maria Luisa Chiofalo
Dip. di Fisica, Università di Pisa & INFN

•

Dott.ssa Giuliana Currò
STMicronics, Rousset

•

Dott. Francesco Pellegrino
Dip. di Fisica e Astronomia, Università di Catania

•

Prof. Alessandro Pluchino
Dip. di Fisica e Astronomia, Università di Catania

•

Prof. Salvatore Savasta
Dip. MIFT, Università di Messina

•

Dott. Vincenzo Savona
Institute of Physics, EPFL, Losanna

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

24 Maggio 2019, ore 15.30, Incubatore d'Impresa Aula HT3-1
V.le F. Stagno d'Alcontres 31, 98166 S. Agata, Messina

Interazione luce-materia in cavità

Dott. Omar Di Stefano
Riken - Wako-shi (Saitama), Japan

Abstract

Lo studio della interazione tra fasci di luce e transizioni atomiche risonanti (alla stessa frequenza) è un problema fondamentale di Fisica della Materia affrontato durante il corso di laurea in Fisica. Come è noto, quando la luce è a bassa intensità la descrizione convenzionale dell'assorbimento dei fotoni è appropriata, ma ad alte intensità il comportamento del sistema cambia drasticamente e si possono osservare le oscillazioni di Rabi. Se i singoli atomi possono essere controllati attraverso tecniche di raffreddamento laser (laser-cooling) o di intrappolamento (trapping), i fotoni possono essere confinati in una cavità con specchi che li riflettono ripetutamente da una parte all'altra agendo quindi come "trappole" per la luce. Al fine di indagare tale problema ad un livello fondamentale è conveniente utilizzare un modello base: un singolo atomo accoppiato ad un singolo quanto di luce (fotone) in un ambiente altamente controllato. Lo scopo di queste lezioni sarà proprio la descrizione di come tale interazione è modificata da una cavità risonante. I limiti dell'accoppiamento atomo-cavità debole (weak-coupling) e forte (strong-coupling) saranno trattati. In particolare, dopo un breve richiamo della teoria della emissione spontanea da atomi liberi nello spazio si descriverà come questo processo viene alterato da una cavità risonante in regime di accoppiamento debole (effetto Purcell). Si introdurrà poi il concetto di accoppiamento forte alla base di diverse importanti applicazioni nel campo delle tecnologie quantistiche di seconda generazione. Più specificatamente, lo strong coupling tra l'atomo e il campo di cavità permette al singolo atomo di controllare la trasmissione di luce in cavità e al singolo fotone di cambiare lo stato dell'atomo. Si discuteranno quindi i modelli di Jaynes-Cummings e di Rabi e loro applicazioni.

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

30 Maggio 2019, ore 15.00, Incubatore d'Impresa Aula HT14
V.le F. Stagno d'Alcontres 31, 98166 S. Agata, Messina

Quattro passi nella Fisica Generale

Prof. Gaetano Saitta

Abstract

Più che di un seminario vero e proprio si tratta di una chiacchierata,...sia pure molto disordinata, su alcuni punti relativi ai contenuti dei corsi storicamente chiamati Fisica I e Fisica II. Vuole essere un "memento" per docenti e studenti su imprecisioni, ingannevoli credenze, leggende metropolitane ed anche qualche suggerimento per affrontare meglio la materia in oggetto che costituisce sempre, a mio avviso, l'ossatura di ogni studioso di fisica.

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

20 Giugno 2019, ore 11.00, Sala seminari, CNR-IPCF
V.le F. Stagno d'Alcontres 37, S. Agata, Messina

A New Era in the Quest for Dark Matter

Prof. Gianfranco Bertone

GRAPPA (Gravitation, AstroParticle Physics Amsterdam) & University of Amsterdam

Abstract

The existence of dark matter has been discussed for more than a century. In the 1970s, astronomers and cosmologists have then began to build what is today a compelling body of evidence for this elusive component of the universe, but the Standard Model of particle physics contains no suitable particle to explain these observations, and thus dark matter arguably represents a glimpse of "new physics". The nature of dark matter remains today poorly constrained, with proposed candidates spanning 90 orders of magnitude in mass, ranging from ultra-light bosons to massive primordial black holes. Here, we discuss what we have learned about the nature of dark matter from past experiments, and the implications for planned dark matter searches in the next decade. We argue that diversifying the experimental effort, incorporating astronomical surveys and gravitational wave observations, is our best hope to make progress on the dark matter problem.

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA
25 Luglio 2019, ore 10.00, Sala seminari, CNR-IPCF
V.le F. Stagno d'Alcontres 37, S. Agata, Messina

Carbon dioxide at geological conditions: from molecular liquid through reactive fluid to polymeric glass

Prof. A. Marco Saitta
Sorbonne Université, Paris, France

Abstract

In this work we propose a full structural and dynamical characterization of carbon dioxide fluids under geological conditions using unprecedented extensive ab initio molecular dynamics amounting to a total 5 ns of simulation time distributed all over the wide pressure and temperature range corresponding to the inferior mantle. We adopt sophisticated structural and dynamical analytical tools to describe the pressure-induced formation of complex chains and the various thermodynamic behaviours encountered. We are able to identify and fully characterize for the first time four different liquid regimes including two distinct polymeric systems and two molecular phases, all within the geothermal conditions of the lower mantle. At lower pressures, we find that the molecular liquid behaviour above 2000 K becomes very reactive, as the C-O bond routinely break and small chains made up of CO₂ briefly form with occasional exchanges of oxygen atoms. At higher pressures, in addition to the polymeric fluid that was previously reported at 3000 K, we find polymeric amorphous behaviour at lower temperature ($T < 2500$ K), which suggests that in this pressure range, the polymeric crystal phase V should dominate, in accordance with previous theoretical work.

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA
2 Ottobre 2019, ore 16.00, Incubatore d'Impresa Aula HT10/11
V.le F. Stagno d'Alcontres 31, 98166 S. Agata, Messina

Dalla fisica alle origini della vita: percorso di un fisico da Messina alla Sorbona

Prof. A. Marco Saitta
Sorbonne Université, Paris, France

Abstract

La fisica è ed è stata spesso considerata il fondamento di tutte le altre discipline scientifiche. Nel corso di questa conferenza cercherò di illustrare come le sue leggi fondamentali, tra cui quelle della meccanica quantistica, possano essere indispensabili anche in campi di ricerca «lontani» dalla fisica stessa. Un esempio illuminante è quello dello studio delle origini della vita, tradizionalmente appannaggio della biologia, della geologia, dell'astronomia, nel quale gli approcci microscopici, basati sulla fisica e sulla chimica, dalla meccanica quantistica alla termodinamica dei processi chimici fuori equilibrio, stanno diventando sempre più importanti. Questa presentazione darà anche modo di illustrare, *en toile de fond*, il mio percorso, cominciato esattamente 30 anni fa come studente in fisica all'Università di Messina, e proseguito, attraverso la SISSA di Trieste, e la University of Pennsylvania di Philadelphia, fino all'Université Pierre et Marie Curie - Sorbona di Parigi, dove ho sviluppato queste ricerche.

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA
30 Ottobre 2019, ore 15.00, Sala seminari, CNR-IPCF
V.le F. Stagno d'Alcontres 37, S. Agata, Messina

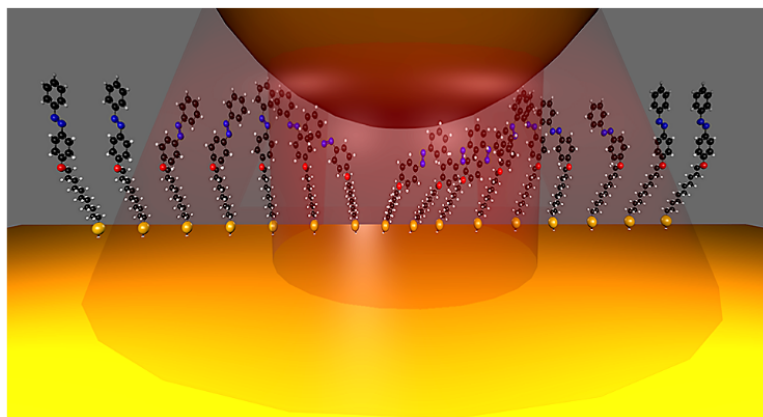
Tip-Enhanced Raman Spectroscopy in Scanning Tunnelling Mode applied to the study of the Molecular Bending in Azobenzene Self-Assembled Monolayers

Dott. Antonino Foti

Dipartimento di Ingegneria dell'Informazione, delle Infrastrutture e dell'Energia Sostenibile (DIIES), Università Mediterranea di Reggio Calabria

Abstract

Tip Enhanced Raman Spectroscopy (TERS) has proven to be a powerful tool for chemical and structural characterization of molecular interfaces at the nanoscale [1]. This technique combines the high chemical specificity of Raman spectroscopy with the high electromagnetic sensitivity provided by huge signal amplification due to the resonant excitation of a plasmonic nanotip. The very end of the tip apex acts like a nanoantenna able to confine and enhance optical fields in a nanometric volume ("hot spot"), thus allowing for the detection of the Raman signal scattered from a small number of molecules. TERS intensity of azobenzene self-assembled monolayers (SAMs) probed in a scanning tunneling mode configuration (STM-TERS), is well described by a physical model that takes into account also the molecular torque induced by the interaction of the high electric field inside the tunneling junction with the molecular dipole [2]. The model predicts quite well the experimental variation in the TERS intensity of a hexil azobenzene SAM (AzoC6) on gold polycrystalline film (111) with changing the electric field inside the gap between the tip and the substrate. Nevertheless, a disagreement between the model and the experiment has been observed while studying, in the same conditions, the TERS intensity of undecyl azobenzene (AzoC11) SAM formed by molecules featuring an alkyl chain nearly two times longer with respect to the previous case. The problem has been solved extending the molecular bending model through considering an additional bending mechanism due to the mechanical interaction between the tip and the SAM, occurring when the tip-to-sample distance is shorter than the molecular length [3].



References

1. Shao F. et al., Analytical and Bioanalytical Chemistry (2019) 411:37–61.
2. Toccafondi C., et al., J Phys. Chem. C, 2016, 120, 18209–18219.
3. Foti A., et al, J Phys. Chem. C, 2019, <https://doi.org/10.1021/acs.jpcc.9b08299>

**DOTTORATO DI RICERCA IN FISICA, SCIENZE CHIMICHE, BIOLOGIA APPLICATA E
MEDICINA SPERIMENTALE DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA**

6 Novembre 2019 - 4 Dicembre 2019

**Serie di seminari su "R&Designing Innovation" organizzati nell'ambito
dell'attività didattica dei Dottorati di Ricerca in: "Fisica", "Scienze Chimiche" e
"Biologia Applicata e Medicina Sperimentale"**

Prof.ssa Donatella Paolino
Università degli Studi di Catanzaro

•

Prof. Stefano Simonella
Università degli Studi di Messina

•

Prof.ssa Daniela Baglieri
Università degli Studi di Messina

•

Ing. Vincenzo Filardi
Università degli Studi di Messina

•

Prof. Giovanni Bottari
Universidad Autonoma de Madrid, Spagna

•

Dott. Paolo Patanè
Università degli Studi di Messina

•

Dott.ssa Alessia Tropea
Università degli Studi di Messina

•

Dott. Francesco Valle
CNR-ISMN, Bologna

•

Prof. Fabio Marino
Università degli Studi di Messina

Abstract

Parte il ciclo di seminari dedicati agli studenti dei Dottorati di Ricerca in «Fisica», «Scienze Chimiche» e «Biologia Applicata e Medicina Sperimentale» dell'Università degli Studi di Messina che punta a favorire le sinergie e la crescita delle competenze gestionali dei "futuri giovani ricercatori/imprenditori" nei settori della ricerca, dello sviluppo imprenditoriale e dell'innovazione. All'interno del nuovo filone formativo dei Dottorati di Ricerca di Area Scientifica, di cui l'Università di Messina è promotore, particolare attenzione viene riservata alla cultura del "saper fare", fornendo strumenti teorici e pratici per la valorizzazione dei risultati della ricerca e per trasformare le idee in risultati economici.

Si inizia col far chiarezza sul concetto di "Trasferimento Tecnologico" che si compone di un insieme di attività finalizzate a portare la conoscenza dalla ricerca al mercato, attraverso attività di sfruttamento della proprietà intellettuale (cessione, licensing, etc.) ed attività di fund raising, con particolare riferimento alla creazione di startup e spin-off accademici.

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

7 Novembre 2019, ore 15.00, Sala seminari, CNR-IPCF
V.le F. Stagno d'Alcontres 37, S. Agata, Messina

Optonanofluidics: bio-inspired soft nanofluidic networks created and controlled by light

Prof. Guido Bolognesi
Department of Chemical Engineering, Loughborough University, UK

Abstract

Liquid transport in flexible nanoconduits is an important process in biological systems, such as organelles and cells. Therefore, artificial soft nanochannel networks are highly desired to mimic their biological counterparts and to investigate the physics and chemistry of these structures. Nevertheless, the creation of such networks can be a relatively difficult task. A well-known fabrication protocol is based on the micro-manipulation, electroporation and micro-injection of polydisperse

giant unilamellar vesicles (GUVs), leading to the creation of lipid nanotubes and daughter vesicles. Although the resulting networks are robust and versatile, this fabrication procedure is quite lengthy (>1hr) and the geometry features of the resulting networks, such as nanotube length and reservoir volume, are poorly controlled. In this lecture, I will present new approaches for the rapid generation of nanofluidic networks based on the optical manipulation of soft structures and particles at liquid interfaces, including i) surfactant-coated ultralow tension droplets and ii) adhesive GUVs. These contactless approaches offer several advantages, including easy implementation, fast (few mins) fabrication of arbitrary complex 2D/3D networks, fine control over network geometry parameters and ability to connect chemically distinct reservoirs (from fL to nL in volume) across distances from 1 μ m to 100s of μ m. Novel experimental methods for the characterisation of the physical properties of these soft structures will be discussed

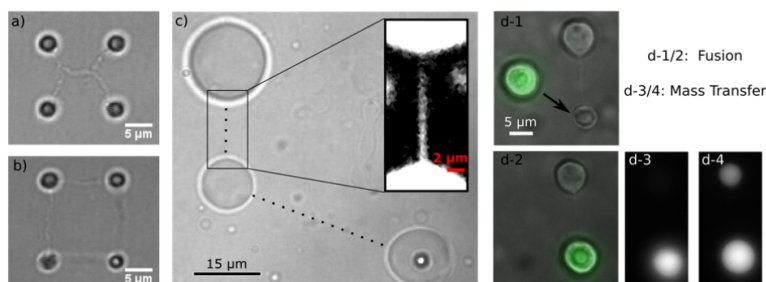


Figure 1: (a-b) Optically trapped drops connected by nanochannels. (c) Surface-immobilised drops connected by nanochannels (dotted lines). (d) Mass transport across a nanochannel

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

19 Novembre 2019, ore 15.00, Sala seminari, CNR-IPCF
V.le F. Stagno d'Alcontres 37, S. Agata, Messina

Prospects for Hadron Spectroscopy

Dr. Alessandro Pilloni

European Center for Theoretical Studies in Nuclear Physics and Related Areas, Trento

Abstract

Quantum Chromodynamics is universally acknowledged as the theory of strong interactions. However, the way how the fundamental constituents (quark and gluons) arrange themselves into the hadrons that are actually observed in experiments, is still a mystery. Even at a phenomenological level, the presence of multiple overlapping states leads to intricate interference patterns that make the extraction of meaningful information complicated. In this colloquium, I will explain what challenges we face every day to understand the spectrum of strong interacting particles. I will review the status of present and planned colliders, and what are the expectations in the near future. I will discuss the role of amplitude analysis in converting the raw experimental data into robust physics information. I will finally show how these tools allow us to solve a longstanding puzzle about the elusive hybrid mesons.

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

5 Dicembre 2019, ore 15.00, Incubatore d'Impresa Aula HT3-1
V.le F. Stagno d'Alcontres 31, 98166 S. Agata, Messina

Lights & shadows of dye-sensitized solar cells

Dr. Giuseppe Calogero

CNR-Istituto per i Processi Chimico Fisici, Messina

Abstract

The recent state of the art of solar devices based on dye-sensitive solar cells (DSSC) will be reviewed. Their design, manufacture and characteristics will be discussed in depth. Here also are analysed the recent advances in the exploitation of natural sensitizers for the conversion of solar energy, comparing them with the synthetic ones. Furthermore, it is provided an in-depth discussion on the main limitation of the use of DSSCs, outlining future developments for their use in large modules, and on some technological solutions which can favour the progress of their integration into living environments and/or in building facades. Finally, I present my point of view on the future prospects of DSSCs also in the field of solar painting art.

DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

12 Dicembre 2019, ore 15.00, Sala seminari, CNR-IPCF
V.le F. Stagno d'Alcontres 37, S. Agata, Messina

Molecular fluorescence: from simple to complex

Dott.ssa Valentina Villari
CNR-Istituto per i Processi Chimico Fisici, Messina

Abstract

The leading idea of the talk, inspired by the results of a recent study on the emission properties of supramolecular complexes between a porphyrin derivative and graphene oxide, is to remind how powerful are the fluorescence-based tools, even the simplest ones as the steady-state and time-resolved spectrofluorimetry, in the study of intermolecular photophysical processes. After a very rapid historical survey of luminescence during the centuries preceding the knowledge of the atomic structure and the development of the quantum theory, the basic concepts describing the main de-activation processes of the molecular excited states are outlined. Among these, the photoinduced electron transfer mechanism is considered and discussed with an example.

PREMI E RICONOSCIMENTI

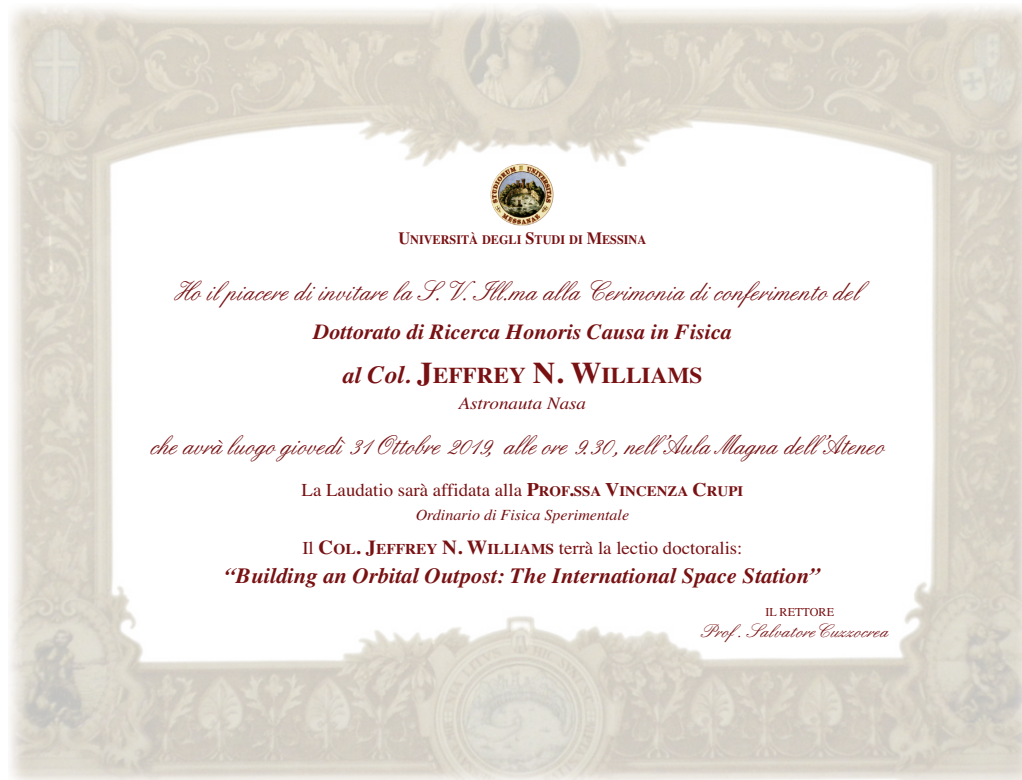
DOTTORATO DI RICERCA IN FISICA DELL'UNIVERSITÀ DEGLI STUDI DI MESSINA

31 Ottobre 2019, ore 9.30, Aula Magna dell'Università Degli Studi di Messina
Piazza Pugliatti, 1, 98122, Messina

Conferimento titolo di Dottore di Ricerca *Honoris Causa* in Fisica al Col. Jeffrey N. Williams, Astronauta NASA da parte dell'Università degli Studi di Messina

La *Laudatio* è stata tenuta dalla Prof.ssa **Vincenza Crupi**
(Coordinatore del Dottorato di Ricerca in Fisica dell'Università degli Studi di Messina)

Motivazione: Jeffrey Williams è laureato in Scienze Applicate e Ingegneria, ed ha conseguito un master in Ingegneria Aeronautica. Ha compiuto svariate missioni spaziali, conseguendo il record di 534 giorni trascorsi nello spazio. Durante la sua attività di astronauta, ha inoltre fornito un significativo apporto tecnico - scientifico, progettando, sviluppando e testando l'upgrade del cockpit dello space shuttle. La proposta di conferimento del *Dottorato Honoris Causa in Fisica* nasce dall'idea di voler, da un lato, riconoscere il merito a chi ha indiscutibilmente contribuito al progresso mondiale, e, dall'altro, di voler valorizzare i possibili sbocchi lavorativi offerti da una preparazione tecnico scientifica, quale quella che viene erogata dal Dipartimento di Scienze Matematiche e Informatiche, Scienze Fisiche e Scienze della Terra (MIFT), nel quale è incardinato il Corso di Dottorato di Ricerca in Fisica.



<https://www.unime.it/it/informa/notizie/conferito-il-dottorato-honoris-causa-fisica-allastronauta-jeffrey-n-williams>

ORGANIZZAZIONE
DEL DOTTORATO DI RICERCA
IN FISICA

Coordinatore: PROF.SSA VINCENZA CRUPI

**Direttore del Dipartimento di Scienze Matematiche e Informatiche,
Scienze Fisiche e Scienze della Terra - Università degli Studi di
Messina: PROF. FORTUNATO NERI**

Segretaria della Scuola di Dottorato: DR.SSA PAOLA DONATO

Delegato per il sito Web del Dipartimento: PROF. ALESSANDRO SERGI

**Piano didattico del Dottorato di Ricerca in Fisica dell'Università
degli Studi di Messina relativo ai Cicli XXXIII e XXXIV
con competenze avanzate in:**

FISICA NUCLEARE E SUBNUCLEARE
FISICA DELLA MATERIA
FISICA APPLICATA

Totale ore Lezioni di Carattere Generale : 90 Ore
Totale minimo di ore di Carattere Specialistico : 60 Ore

150 ore minime in Totale per Dottorando.

***** Area di Fisica Nucleare e Subnucleare *****
REFERENTI PROFF.RI A. TRIFIRÒ E G. MANDAGLIO

Lezioni di interesse generale (12 ore):

1. Dinamica delle Reazioni Nucleari (4 ore);
2. Risonanze barioniche e sezioni d'urto adroniche (4 ore);
3. Fisica delle particelle con sonde elettromagnetiche e leptoniche (4 ore);

Lezioni di Interesse Specialistico (Moduli ciascuno di 10 ore; tot. 80 ore):

1. Teoria delle Reazioni Nucleari;
2. Reazioni di multiframmentazione o formazione di nuclei superpesanti;
3. Teoria delle Interazioni Fondamentali;
4. Fasci Ionici in Plasmi prodotti da Laser;
5. Rivelazione e analisi dei prodotti di reazione in Fisica Nucleare, Subnucleare e Astrofisica;
6. Risonanze barioniche e sezioni d'urto adroniche in Fisica delle Particelle;
7. Acquisizione, elaborazione dei dati e procedure di simulazione nei processi nucleari;
8. Emissione di fotoni e particelle in processi nucleari;

***** Area di Fisica della Materia *****
Aspetti Teorici
REFERENTE PROF. S. G. PRESTIPINO

Lezioni di interesse generale (12 ore):

1. Fisica Teorica e Computazionale dello stato liquido della materia.

Lezioni di Interesse Specialistico (Moduli ciascuno di 10 ore, tot. 50 ore):

1. Formazione di aggregati in fluidi con interazioni microscopiche antagoniste;
2. Comportamento di fase complesso in sistemi caratterizzati da interazioni semplici;
3. Teoria della nucleazione di solidi cristallini da fasi liquide;
4. Simulazioni numeriche di liquidi a legame idrogeno;
5. Simulazione della dinamica quantistica dissipativa.

***** Area di Fisica della Materia *****
Fisica dei sistemi Disordinati
REFERENTE PROF.SSA G. D'ANGELO

Lezioni di interesse generale (12 ore):

1. Disordine e Localizzazione (4 ore)
2. La transizione vetrosa (4 ore)
3. Dinamica Ionica in sistemi disordinati (4 ore)

Lezioni di Interesse Specialistico (Moduli ciascuno di 10 ore, tot. 30 ore):

1. Dinamica vibrazionale e rilassamenti in solidi amorfi;
2. Spettroscopia dielettrica in materiali a conduzione ionica;
3. Spettroscopia Meccanica in polimeri.

***** Area di Fisica della Materia *****
Nanosistemi e Fotonica
REFERENTE PROF. F. NERI

Lezioni di interesse generale (12 ore):

1. Materiali nano strutturati (4 ore);
2. Sistemi quantistici complessi (4 ore);
3. Nano-Ottica (4 ore).

Lezioni di Interesse Specialistico (Moduli ciascuno di 24 ore, tot. 72 ore):

1. Nanomateriali e dispositivi:
 - Sintesi di nano sistemi (8 ore);
 - Materiali a bassa dimensionalità (8 ore);
 - Plasmonica e SERS (8 ore).
2. Diagnostica di nano e microsistemi:

- Micro-imaging (8 ore);
 - Spettroscopia Elettronica (8 ore);
 - Microscopia (8 ore);
3. Processi fisici su scala nanometrica:
- Fotonica (8 ore);
 - Intrappolamento ottico (8 ore);
 - Scattering ed assorbimento di luce (8 ore).

*** Area di Fisica della Materia ***

Biofisica

REFERENTI PROFF.RI S. MAGAZÙ E D. MAJOLINO

Lezioni di interesse generale (10 ore):

1. La visione moderna della biofisica molecolare: organizzazione della materia biologica e termodinamica dei processi biologici (5 ore);
2. Caratterizzazione strutturale e dinamica di sistemi di interesse biofisico mediante tecniche spettroscopiche complementari e tecniche simulative (5 ore).

Lezioni di Interesse Specialistico (Tot. Moduli 50 ore):

1. Proprietà chimico-fisiche delle biomolecole e influenza del solvente (e.g. folding, unfolding e misfolding delle proteine, etc...) (5 ore).
2. Caratterizzazione strutturale di sistemi di interesse biofisico (e.g. macromolecole, membrane, etc...) mediante tecniche PCS, SANS/SAXS, X-Radial Diffraction, NMR, microscopia e spettrometria di massa (15 ore).
3. Caratterizzazione dinamica di sistemi di interesse biofisico (e.g. macromolecole biologiche, sistemi host-guest, idrogels, etc...) mediante spettroscopia Raman e IR (10 ore).
4. Scattering elastico, quasi-elastico e anelastico di neutroni per la caratterizzazione dinamica di sistemi di interesse biofisico (e.g. polisaccaridi, proteine, etc...) (10 ore).
5. Tecniche calorimetriche e reologiche per la caratterizzazione di sistemi di interesse biofisico (5 ore).
6. Caratterizzazione strutturale e dinamica di sistemi di interesse biofisico mediante metodi computazionali (5 ore).

*** Area di Fisica della Materia e Area di Fisica Nucleare ***

Fisica dei Plasmi

REFERENTE PROF. L. TORRISI

Lezioni di interesse generale (4 ore):

1. Plasmi LTE e NLTE e Fisica Sperimentale associata (4 ore).

Lezioni di Interesse Specialistico (Tot. Moduli 16 ore):

1. Tecniche Diagnostiche di plasmi laser (6 ore);
2. Laser ion sources (5 ore);
3. Laser particle acceleration (5 ore).

***** Area di Fisica Applicata *****
Fisica Applicata ai Beni Culturali, Ambientali e Medicina
REFERENTI PROF. RI D. MAJOLINO, S. MAGAZÙ, L. TORRISI

Lezioni di interesse generale (12 ore):

1. Le tecniche spettroscopiche nel campo dei Beni Culturali (10 ore);
2. Monitoraggio Ambientale (2 ore).

Lezioni di Interesse Specialistico (Tot. Moduli 22 ore) :

1. Diffrazione di neutroni per la caratterizzazione microscopica di reperti archeologici (2 ore);
2. Lo scattering di neutroni a piccolo angolo per la caratterizzazione mesoscopica di reperti archeologici (2 ore);
3. L'assorbimento di raggi X da luce di sincrotrone per la caratterizzazione superficiale di reperti archeologici (2 ore);
4. Spettroscopia a raggi X-caratteristici (4 ore);
5. Spettrometria di massa (2 ore);
6. Tecnica LAMQS (Laser Ablation coupled to Mass Quadrupole Spectrometry) (4 ore);
7. Analisi e Trattamento di Materiali biocompatibili (2 ore);
8. Tecniche di monitoraggio inquinamento dell'aria ed elettromagnetico (4 ore).

***** Area di Fisica Applicata*****
Geofisica
REFERENTE PROF. G. NERI

Lezioni di interesse generale (4 ore):

1. Ricerche di geofisica e geodinamica nella regione calabro-peloritana e nel complesso Tirreno-Ionio (2 ore);
2. Studi della sismicità e della pericolosità sismica con particolare riferimento all'impiego di metodologie fisiche (2 ore).

Lezioni di Interesse Specialistico (Moduli ciascuno di 9 ore, tot. 18 ore):

1. Geofisica (9 ore);
2. Sismologia (9 ore).

OFFERTA FORMATIVA CICLO XXXV

Anno Accademico 2019-2020

6 Posti ciascuno con borsa di studio

Una delle 6 borse di studio è stata assegnata su progetto finanziato nell'ambito del Programma Operativo Complementare Ricerca e Innovazione 2014 – 2020 (POC R&I), Asse Tematico 1 “Capitale Umano” – Azione I.1 “Dottorati Innovativi con caratterizzazione industriale”

ATTIVITÀ DI FORMAZIONE

Linguistica: Si prevedono attività formative in lingua Inglese finalizzate a facilitare la stesura della tesi finale in inglese e ad incentivare le molteplici collaborazioni scientifiche internazionali peculiari del percorso di dottorato. Infine, è ormai consolidata l'organizzazione di una “giornata di studio” in occasione della quale i dottorandi sono invitati a redigere in inglese un lavoro sul Report Annuale (ISSN 2038-5889) del DdR in Fisica riguardante l'attività di ricerca svolta annualmente.

Informatica: Si prevedono attività formative di inizializzazione informatica presso il nostro Ateneo, finalizzate a fornire ai dottorandi abilità nell'utilizzo di linguaggi di scrittura come il sistema LATEX per la preparazione di testi scientifici, nell'utilizzo dell'architettura GRID e di calcolo parallelo per l'elaborazione di grandi set di dati.

Gestione della ricerca, della conoscenza dei sistemi di ricerca e dei sistemi di finanziamento: Si prevede una serie di seminari specialistici da parte di esperti del settore inerenti la gestione della ricerca a livello nazionale ed internazionale, il coordinamento di gruppi di ricercatori e le modalità di ricerca dei canali di finanziamento nazionali ed internazionali al fine di fornire ai dottorandi le giuste abilità per la stesura di progetti di finanziamento anche internazionali.

Valorizzazione dei risultati della ricerca e della proprietà intellettuale: Si prevedono seminari specialistici inerenti la valorizzazione dei risultati della ricerca e della proprietà intellettuale. Saranno svolti da docenti coinvolti in esperienze di ricerca nazionale ed internazionale, nonché da personale docente e/o funzionari delle strutture di Ateneo operante nel campo dell'attrazione di risorse e della valorizzazione della proprietà intellettuale.

OFFERTA FORMATIVA E ARTICOLAZIONE IN CFU

L'impegno complessivo è di 180 crediti formativi, distribuiti uniformemente sui tre anni di corso (60 CFU per ogni singolo anno). Nello specifico, i crediti formativi saranno così distribuiti:

I ANNO

- Cicli di lezioni e attività formativa specialistica (n. 18 CFU).
- Attività individuale di ricerca da discutere per il passaggio all'anno successivo al primo (n. 23 CFU).
- Redazione in lingua inglese dell'attività di ricerca svolta nel volume del report annuale del DdR in Fisica (Activity Report, ISSN 2038-5889) (n. CFU 10).
- Partecipazione a seminari, congressi, scuole, soggiorni all'estero e in Italia (n. max CFU 10).
- Attività a scelta libera (n. max CFU 8).

II ANNO

- Attività individuale di ricerca da discutere per il passaggio all'anno successivo al secondo (n. 23 CFU).
- Redazione in lingua inglese dell'attività di ricerca svolta nel volume del report annuale del DdR in Fisica (Activity Report, ISSN 2038-5889) (n. CFU 10).
- Partecipazione a seminari, congressi, scuole, soggiorni all'estero e in Italia, presentazione di contributi sotto forma di abstract, poster o come relatore (n. max CFU 25).
- Attività a scelta libera (n. max CFU 8).

III ANNO

- Stesura tesi e relativa discussione (n. CFU 35).
- Attività individuale di ricerca da discutere per l'ammissione all'esame finale (n. 23 CFU).
- Attività a scelta libera (n. max CFU 8).

Legenda per l'attribuzione dei crediti alle attività formative a scelta

- Soggiorno di ricerca all'estero di tipo Erasmus o di altro tipo del dottorando, sarà valutata dal consiglio dei docenti ai fini dell'attribuzione dei crediti formativi e della sua quantificazione
- La frequenza di corsi di specializzazione o di attività formative certificabili connesse con l'attività formativa e di ricerca del dottorando sarà valutata dal consiglio dei docenti ai fini dell'attribuzione dei crediti formativi e della sua quantificazione
- La pubblicazione di articoli scientifici su rivista, di saggi in volume, di capitoli di libro o di monografia, per la quale farà fede la data di accettazione del contributo o la pubblicazione del volume, sarà valutata dal consiglio dei docenti ai fini dell'attribuzione dei crediti formativi e della sua quantificazione
- L'attività di tutorato degli studenti nei corsi di Laurea e Laurea magistrale dell'Università Messina sarà valutata dal consiglio dei docenti ai fini dell'attribuzione dei crediti formativi e della sua quantificazione
- L'attività di didattica integrativa sarà valutata dal consiglio dei docenti ai fini dell'attribuzione dei crediti formativi e della sua quantificazione. Si precisa che le attività formative a scelta non possono superare la totalità di 8 CFU per ogni singolo anno di corso. I crediti formativi in esubero, dunque, non saranno computati ai fini del raggiungimento della soglia annua.

CARATTERE INTERNAZIONALE DEL DOTTORATO

Alcuni fra i principali Atenei e centri di ricerca internazionali con i quali i componenti del collegio dei docenti intrattengono collaborazioni di ricerca:

- Academy of Science of Czech Republic (ASCR) and PALS Laboratory of Prague (Repubblica Ceca)
- Rutherford Appleton Laboratory, Didcot-Oxfordshire (UK)
- Budapest Neutron Centre, Budapest (Ungheria)
- Joint Institute for Nuclear Research, Dubna (Russia)
- University of Bonn, Bonn (Germania)
- University of Novosibirsk, Novosibirsk (Russia)

- Budker Institute for Nuclear Physics, Novosibirsk (Russia)
- Institut Laue-Langevin (ILL) Grenoble (Fr)
- Laboratoire Léon Brillouin (LLB), Saclay (Fr)
- ESRF – European Synchrotron Radiation Facility, Grenoble (Fr)
- CERN, Ginevra (CH)
- IPPLM, Warsaw (PL)
- Military University of Technology (MUT), Warsaw (PL)
- Centro di Ricerca RIKEN (Giappone).

COLLEGIO DEI DOCENTI
DEL DOTTORATO DI RICERCA
IN FISICA

Collegio dei Docenti del Dottorato di Ricerca in Fisica Cicli XXXIII e XXXIV

Docente

1. Corsaro Carmelo
2. Costa Dino
3. Crupi Vincenza
4. Cutroneo Mariapompea
5. D'Angelo Giovanna
6. Fazio Enza
7. Finocchio Giovanni
8. Gucciardi Pietro
9. Magazù Salvatore
10. Majolino Domenico
11. Mandaglio Giuseppe
12. Maragò Onofrio
13. Mezzasalma Angela Maria
14. Micali Norberto
15. Neri Fortunato
16. Neri Giancarlo
17. Orecchio Barbara
18. Patanè Salvatore
19. Prestipino Giarritta Santi
20. Puglisi Rosaria Anna
21. Saija Franz
22. Saija Rosalba
23. Savasta Salvatore
24. Torrisi Lorenzo
25. Trifirò Antonio
26. Trimarchi Marina
27. Trusso Sebastiano
28. Venuti Valentina
29. Wanderlingh Ulderico

e-mail

ccorsaro@unime.it
dcosta@unime.it
vincenza.crupi@unime.it
cutroneo@ujf.cas.cz
gdangelo@unime.it
enfazio@unime.it
giovanni.finocchio@unime.it
Gucciardi@me.cnr.it
smagazu@unime.it
domenico.majolino@unime.it
giuseppe.mandaglio@unime.it
marago@me.cnr.it
angelamaria.mezzasalma@unime.it
micali@me.cnr.it
fortunato.neri@unime.it
giancarlo.neri@unime.it
barbara.orecchio@unime.it
salvatore.patane@unime.it
sprestipino@unime.it
rosaria.puglisi@imm.cnr.it
saija@me.cnr.it
rosalba.saija@unime.it
salvatore.savasta@unime.it
lorenzo.torrisi@unime.it
atrifiro@unime.it
marina.trimarchi@unime.it
trusso@me.cnr.it
valentina.venuti@unime.it
ulderico.wanderlingh@unime.it

Collegio dei Docenti del Dottorato di Ricerca in Fisica Ciclo XXXV

Docente

1. Branca Caterina
2. Corsaro Carmelo
3. Costa Dino
4. Crupi Vincenza
5. Cutroneo Mariapompea
6. D'Angelo Giovanna
7. Fazio Enza
8. Gucciardi Pietro
9. Magazù Salvatore
10. Majolino Domenico
11. Mandaglio Giuseppe
12. Maragò Onofrio
13. Micali Norberto
14. Neri Fortunato
15. Orecchio Barbara
16. Patanè Salvatore
17. Presti Debora
18. Prestipino Giarritta Santi
19. Puglisi Rosaria Anna
20. Saija Franz
21. Saija Rosalba
22. Savasta Salvatore
23. Sergi Alessandro
24. Torrisi Lorenzo
25. Trifirò Antonio
26. Trimarchi Marina
27. Trusso Sebastiano
28. Venuti Valentina
29. Wanderlingh Ulderico

e-mail

cbranca@unime.it
ccorsaro@unime.it
dcosta@unime.it
vincenza.crupi@unime.it
cutroneo@ujf.cas.cz
gdangelo@unime.it
enfazio@unime.it
Gucciardi@me.cnr.it
smagazu@unime.it
domenico.majolino@unime.it
giuseppe.mandaglio@unime.it
marago@me.cnr.it
micali@me.cnr.it
fortunato.neri@unime.it
barbara.orecchio@unime.it
salvatore.patane@unime.it
dpresti@unime.it
sprestipino@unime.it
rosaria.puglisi@imm.cnr.it
saija@me.cnr.it
rosalba.saija@unime.it
salvatore.savasta@unime.it
alessandro.sergi@unime.it
lorenzo.torrisi@unime.it
atrifiro@unime.it
marina.trimarchi@unime.it
trusso@me.cnr.it
valentina.venuti@unime.it
ulderico.wanderlingh@unime.it

TESI ED ARGOMENTI
DI RICERCA
STUDENTI DEL DOTTORATO
DI RICERCA IN FISICA

Tesi degli Studenti del Dottorato di Ricerca in Fisica Ciclo XXXII

DOTTORANDO	TITOLO DELLA TESI	TUTOR CO-TUTOR
Dr. Costa Giuseppe gcosta@unime.it	Ion Acceleration by High Intensity Pulsed Laser: Transport, Diagnostics and Theoretical Modelling	Prof. L. Torrisi
Dr. Paladini Giuseppe gpaladini@unime.it	Branched polyethyleneimine/TEMPO-oxidized cellulose nanofibers xerogels for water remediation: a structural and dynamical study by small angle neutron scattering (SANS) and Fourier-transform infrared spectroscopy (FTIR).	Prof.ssa V. Venuti Prof.ssa V. Crupi
Dr. Romano Valentino vromano@unime.it	Two-dimensional materials for energy storage and generation	Prof.ssa G. D'Angelo Dr. F. Bonaccorso Prof. Giulia Grancini
Dr.ssa Medlej Israa imedlej@unime.it	Micromagnetic modeling of skyrmion dynamics and THz oscillation in antiferromagnets	Prof. G. Finocchio

VALUTATORI dei lavori di TESI

DOTTORANDO	REFEREE
Dr. Costa Giuseppe	1) Dr. Ing. Jan Pšikal, <i>Department of Physical Electronics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Czech Republic</i> 2) Dr. Marcin Rosiński, <i>Institute of Plasma Physics and Laser Microfusion (IPPLM), Hery St. 23, 00-908 Warsaw, Poland</i>
Dr. Paladini Giuseppe	1) Prof. Carlo Punta, <i>Department of Chemistry, Materials, and Chemical Engineering "G. Natta", Politecnico di Milano, Via Mancinelli 7, 20131 Milano, Italy and INSTM Local Unit</i> 2) Dr. Jose Teixeira, <i>Laboratoire Léon Brillouin, UMR12 CEA-CNRS, Bât. 563 CEA Saclay, France</i>
Dr. Romano Valentino	1) Prof. Aldo Di Carlo, <i>Dept. Electronic Engineering, University of Rome "Tor Vergata," via del Politecnico 1, 00133 Roma</i> 2) Prof. Emmanuel Kymakis, <i>Department of Electrical & Computer Engineering, Hellenic Mediterranean University, Estavromenos, Heraklion, GR-71410, Crete, Greece</i>
Dr.ssa Medlej Israa	1) Dr.ssa Paola Tiberto, <i>INRIM (Torino) - Str. delle Cacce, 91, 10135 Torino TO, Italy</i> 2) Prof. Mario Carpentieri, <i>Politecnico di Bari, Via E. Orabona 4, I-70125 Bari</i>

**Argomenti di Ricerca del Dottorato in Fisica
Cicli XXXIII, XXXIV**

CICLO XXXIII		
DOTTORANDO	ARGOMENTO DI RICERCA	TUTOR & CO-TUTOR
Dr. Calabretta Cristiano ccalabretta@unime.it	Studio dei processi di impiantazione ionica ed annealing nei MOSFET di potenza in SiC	Prof. L. Torrisi Prof.ssa L. Calcagno
Dr.ssa Longo Sveva sveva.longo@unime.it	Diagnostica di opere d'arte lignee di interesse storico-artistico mediante TC, MRI, micro-NMR e FTIR	Prof.ssa E. Fazio Prof.ssa S. Capuani
Dr. Patti Francesco fpatti@unime.it	Studio teorico dell'interazione tra radiazione elettromagnetica e nanomateriali	Prof.ssa R. Saija
Dr. Settineri Alessio alesettineri@unime.it	Sistemi quantistici ibridi aperti in regime di interazione ultra-forte	Prof. S. Savasta

CICLO XXXIV		
DOTTORANDO	ARGOMENTO DI RICERCA	TUTOR & CO-TUTOR
Dr. Giovanni Borgh gborgh@unime.it	Drogaggio molecolare di nanofili di silicio (SiNWs) per celle solari	Prof. S. Patanè Dott.ssa R.A. Puglisi
Dr. Sergio Gurgone sgurgone@unime.it	Studio dell'adattamento biomeccanico mediante metodologie fisiche	Prof.ssa V. Venuti Dott. G. Aciri
Dr.ssa Bruna Mazza bruna.mazza93@gmail.com	Problematiche riguardanti l'affidabilità dei dispositivi in carburo di silicio	Prof. S. Patanè
Dr. Daniele Pistone daniele.pistone@hotmail.it	Produzione delle risonanze $K^*(892)$ e $\Sigma^*(1385)$ con l'esperimento ALICE a LHC	Prof. G. Mandaglio Dott.ssa A. Badalà
Dr. Paolo Polimeno polimenop@unime.it	Teoria dello scattering elettromagnetico alla nano- e micro-scala	Prof.ssa R. Saija Dott. O.M. Maragò Dott.ssa M.A. Iati
Dr. Davide Romano dromano@unime.it	Natural radioactivity from Radon in northeastern Sicily: application, measurement and continuous monitoring	Prof. Salvatore Magazù Dott. Francesco Italiano Dott. Giuseppe Sabatino

PUBBLICAZIONI
DEGLI
STUDENTI DEL DOTTORATO
DI RICERCA IN FISICA
2019

PUBBLICAZIONI 2019 XXXIII Ciclo

Cristiano Calabretta

1. M. ZIMBONE, M. ZIELINSKI, E. BARBAGIOVANNI, C. CALABRETTA, F. LA VIA, “*3C-SiC grown on Si by using a Si_{1-x}Ge_x buffer layer*”, Jour. of Crystal Growth **519**, 1-6 (2019)
2. C. CALABRETTA, M. AGATI, M. ZIMBONE, S. BONINELLI, A. CASTIELLO, A. PECORA, G. FORTUNATO, L. CALCAGNO, L. TORRISI, F. LA VIA, “*Laser Annealing of P and Al implanted 4H-SiC epitaxial layers*”, Materials **12**, 3362 (2019)
3. M. ZIMBONE, M. ZIELINKY, C. BONGIORNO, C. CALABRETTA, R. ANZALONE, S. SCALESE, A. LA MAGNA, F. MANCARELLA, F. LA VIA, “*3C-SiC growth on Inverted Silicon Pyramids patterned substrate*”, Materials **12**, 3407 (2019)
4. R. ANZALONE, M. ZIMBONE, C. CALABRETTA, M. MAUCERI, A. ALBERTI, R. REITANO, F. LA VIA, “*Temperature investigation on 3C-SiC homo-epitaxy on 4 inches wafers*”, Materials **12**, 3293 (2019)
5. P. BADALÀ, S. RASCUNÀ, B. CAFRA, A. BASSI, E. SMECCA, M. ZIMBONE, C. BONGIORNO, C. CALABRETTA, F. LA VIA, F. ROCCAFORTE, M. SAGGIO, G. FRANCO, A. MESSINA, A. LA MAGNA, “*Ni/4H-SiC interaction and silicide formation under excimer laser annealing for ohmic contact*”, Materialia **9**, 100528 (2019)
6. C. CALABRETTA, M. ZIMBONE, E. G. BARBAGIOVANNI, S. BONINELLI, N. PILUSO, A. SEVERINO, M. A. DI STEFANO, S. LORENTI, L. CALCAGNO, F. LA VIA, “*Thermal Annealing of high dose P implantation 4H-SiC epitaxial layers*”, Mat. Sci. Forum **963**, 399-402 (2019)
7. A. SEVERINO, D. MELLO, S. BONINELLI, F. ROCCAFORTE, F. GIANNAZZO, P. FIORENZA, C. CALABRETTA, L. CALCAGNO, N. PILUSO, G. ARENA, “*Effect of thermal annealing processes in Phosphorus implanted 4H-SiC layers*”, Mat. Sci. Forum **963**, 407-411 (2019)

Sveva Longo

1. G. FORNACIARI, S. MARINOZZI, D. MESSINEO, C. CALDARINI, F. ZAVARONI, S. IORIO, S. LONGO, S. CAPUANI, P. CATALANO, V. GAZZANIGA, “*A remarkable case of gout in the Imperial Rome. Surgery and diseases in Antiquity by osteoarchaeological, paleopathological and historical perspectives*”, International Journal of Osteoarchaeology (2019)
2. G. FESTA, G. SANCESARIO, C. CORSARO, S. LONGO, D. MALLAMACE, E. FAZIO, L. ARCIDIACONO, V. GARCIA SAKAI, R. SENESI, G. SANCESARIO, F. MALLAMACE, C. ANDREANI, “*SANS study of Amyloid β 140: Unfolded monomers in DMSO, multidimensional aggregates in water medium*”, Physica A: Statistical Mechanics and its Applications (2019)

Francesco Patti

1. F. PATTI, R. SAIJA, P. DENTI, G. PELLEGRINI, P. BIAGIONI, M. A. IATI, O. M. MARAGO, “*Chiral optical tweezers for optically active particles in the T-matrix formalism*”, Nature Scientific Reports (2019)

Alessio Settineri

1. O. DI STEFANO, A. SETTINERI, V. MACRÌ, L. GARZIANO, R. STASSI, S. SAVASTA, F. NORI, “*Resolution of gauge ambiguities in ultrastrong-coupling cavity quantum electrodynamics*”, Nature Physics, **1** (2019)
2. C. TRIOLO, S. SAVASTA, A. SETTINERI, S. TRUSSO, R. SAIJA, N. R. AGARWAL, S. PATANÈ, “*Near-field imaging of surface-plasmon vortex-modes around a single elliptical nanohole in a gold film*”, Scientific reports **9**, 5320 (2019)
3. O. DI STEFANO, A. SETTINERI, V. MACRÌ, A. RIDOLFO, R. STASSI, A. F. KOCKUM, S. SAVASTA, F. NORI, “*Interaction of mechanical oscillators mediated by the exchange of virtual photon pairs*”, Physical review letters **122**, 030402 (2019)
4. A. SETTINERI, V. MACRÌ, L. GARZIANO, O. DI STEFANO, F. NORI, S. SAVASTA , “*Conversion of mechanical noise into correlated photon pairs: Dynamical Casimir effect from an incoherent mechanical drive*”, Phys. Rev. A **100**, 022501 (2019)

PUBBLICAZIONI 2019 XXXIV Ciclo

Giovanni Borgh

1. R.A. PUGLISI, C. BONGIORNO, G. BORGH, E. FAZIO, C. GAROZZO, G. MANNINO, F. NERI, G. PELLEGRINO, S. SCALESE AND A. LA MAGNA, "Study on the Physico-Chemical Properties of the Si Nanowires Surface", *Nanomaterials*, **9**, ISSN 2079-4991 (2019)

Sergio Gurgone

1. BORZELLI D., GURGONE S., DE PASQUALE P., BERGER D.J., D'AVELLA .A, "Consistency of Myoelectric Control Across Multiple Sessions". In: Masia L., Micera S., Akay M., Pons J. (eds) *Converging Clinical and Engineering Research on Neurorehabilitation III*. ICNR 2018. *Biosystems & Biorobotics*, vol **21**. Springer, Cham (2019)
2. SALMERI F. M., DENARO L., RUELLO E., ACRI G., GURGONE S., SANSOTTA C., TESTAGROSSA B., "Irradiation with Polychromatic Incoherent Low Energy Radiation of Human Peripheral Blood Mononuclear Cells in vitro Effects on Cytokine Production". *International Journal of Environmental Research and Public Health* (submitted)
3. ACRI G., GURGONE S., SANSOTTA C., DENARO L., RUELLO E., TESTAGROSSA B., "Telethermographic Monitoring of MRI Coils During Quality Controls". *Journal of Imaging* (submitted)

Daniele Pistone

1. BY ALICE COLLABORATION (SHREYASI ACHARYA ET AL.), "Measurement of $\Upsilon(1S)$ elliptic flow at forward rapidity in Pb-Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV", arXiv:1907.03169 [nucl-ex]. 10.1103/PhysRevLett.123.192301. *Phys. Rev. Lett.* **123**, no.19, 192301 (2019).
2. BY ALICE COLLABORATION (SHREYASI ACHARYA ET AL.), " ${}^3_{\Lambda}\text{H}$ and ${}^3_{\Lambda}\bar{\text{H}}$ lifetime measurement in Pb-Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV via two-body decay", arXiv:1907.06906 [nucl-ex]. 10.1016/j.physletb.2019.134905. *Phys. Lett. B* **797**, 134905 (2019).

Paolo Polimeno

1. POLIMENO, R. SAIJA, C. DEGLI ESPOSTI BOSCHI, O. M. MARAGÒ, M. A. IATÌ, "Optical forces in the Tmatrix formalism", *Atti della Accademia Peloritana dei Pericolanti* **1:A2**, (2019)

Davide Romano

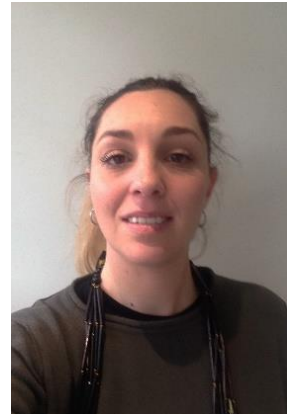
1. F. ITALIANO, D. ROMANO, C. CARUSO, M. LONGO, A. CORBO, G. LAZZARO, "*Magmatic Signature in Submarine Hydrothermal Fluids Vented Offshore Ventotene and Zannone Islands (Pontine Archipelago, Central Italy)*", *Geofluids*, **2019**, Article ID 8759609 (2019)
2. G. SABATINO, M. DI BELLA, F. CARIDI, F. ITALIANO, D. ROMANO, S. MAGAZÙ, A. GNISCI, G. FAGGIO, G. MESSINA, S. SANTANGELO, F. LEONETTI, A. TRIPODO, "*Radiological assessment, mineralogy and geochemistry of the heavy-mineral placers from the Calabrian coast (South Italy)*", *Journal of Instrumentation*, **14**, (2019)
3. D. ROMANO, A. GATTUSO, M. LONGO, C. CARUSO, G. LAZZARO, A. CORBO, F. ITALIANO, "*Hazard Scenarios related to submarine volcanic-hydrothermal activity and advanced monitoring strategies: study case from the Panarea volcanic group (Aeolian Islands, Italy)*", *Geofluids* Vol. **2019**, Article ID 8728720 (2019)

GALLERIA FOTOGRAFICA
DEGLI
STUDENTI DEL DOTTORATO
DI RICERCA IN FISICA
2019

Studenti di Dottorato Ciclo XXXIII



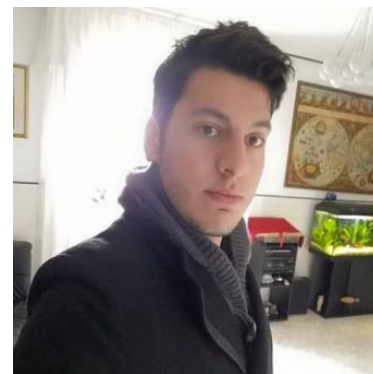
Cristiano Galabretta



Sveva Longo



Francesco Zatti



Alessio Settinieri

Studenti di Dottorato Ciclo XXXIV



Giovanni Borgh



Sergio Gurgone



Bruna Mazza



Daniele Distone



Paolo Polimeno



Davide Romano

Studenti di Dottorato Ciclo XXXV



Laura Anoldo



Letterio Biondo



Giovanni Gallo



Rosa Musotto



Antonina Rosano



Abir Saidi

ALTA FORMAZIONE
E
RICERCA SCIENTIFICA

Alta Formazione e Ricerca Scientifica Via Consolato del Mare 41 (Palazzo Mariani)

Dottorati di Ricerca

I Corsi di Dottorato di Ricerca hanno la finalità di fornire agli iscritti competenze di alto livello e qualificazione scientifica, acquisite mediante attività di formazione alla ricerca e di didattica strutturata, necessarie all'esercizio di mansioni di ricerca e di elevata professionalità presso Enti pubblici e privati, rappresentano, pertanto, il terzo livello degli studi universitari.

I Corsi di Dottorato hanno durata triennale/quadriennale e prevedono la frequenza obbligatoria. Requisito di ammissione è il possesso della Laurea Specialistica e/o Magistrale o il Diploma di Laurea conseguito prima dell'entrata in vigore del D.M.5009/99 ovvero di altro titolo di studio conseguito all'estero e riconosciuto idoneo, oltre il superamento delle prove di esame previste dai Bandi di concorso emanati dall'Università e pubblicati nella Gazzetta Ufficiale della Repubblica Italiana.

Almeno la metà dei posti messi a concorso è coperta da borse di studio in parte finanziate dal MIUR e dall'Ateneo, in parte da altre Università o Enti esterni pubblici o privati.

Il titolo di Dottore di Ricerca si consegue all'atto del superamento dell'esame finale che consiste nella discussione della Tesi di Dottorato e che può essere ripetuto una sola volta.

È possibile, inoltre, ottenere una certificazione di "Doctor Europaeus" - aggiuntiva al titolo nazionale del dottorato - nel rispetto delle condizioni richieste dall'European University Association, in seguito ad un soggiorno di ricerca di almeno un trimestre, anche non continuativo, in una struttura di un altro Paese dell'Unione Europea.

<https://www.unime.it/it/ricerca/dottorati-ricerca/contatti-dottorati-di-ricerca>

Post-Dottorato di Ricerca

Le borse di studio post-dottorato vengono assegnate, con un concorso per titoli, ai possessori del titolo di Dottore di Ricerca.

Hanno una durata biennale e prevedono un'attività di ricerca da svolgersi non solo in strutture dell'Università di Messina ma anche presso i laboratori stranieri con i quali siano in corso attività di collaborazione.

Perfezionamento Estero

Le borse di perfezionamento estero hanno una durata annuale e vengono assegnate, con un concorso per titoli ed esami, ai possessori della Laurea Specialistica e/o Magistrale o il Diploma di Laurea conseguito prima dell'entrata in vigore del D.M.5009/99 ovvero di altro titolo di studio conseguito all'estero e riconosciuto idoneo; di età inferiore ai 29 anni che documentino un impegno formale di attività di perfezionamento presso istituzioni estere o internazionali di livello universitario.

Borse Private

Le borse private, o alla memoria, vengono finanziate da soggetti privati esterni all'Università e prevedono anch'esse lo svolgimento di un particolare progetto di ricerca specificato nel bando di concorso.

UNITÀ DI COORDINAMENTO TECNICO
Via Consolato del Mare 41 (Palazzo Mariani)

Responsabile

Ing. Carlo Costanzo
ccostanzo@unime.it – 090 676 8909

Staff

Sig.ra Rosita Di Perna
rdiperna@unime.it – 090 676 8502

UNITA' ORGANIZZATIVA SERVIZI ALLA RICERCA

Responsabile

Dott.ssa Maria Pia Mangano
mpmangano@unime.it – 090 676 8503

UNITA' OPERATIVA "DOTTORATI DI RICERCA"

Responsabile

Dott.ssa Angelina Venezia
avenezia@unime.it – 090 676 8716

Vice Responsabile

Dott.ssa Angela Garozzo
agarozzo@unime.it – 090 676 8505

Staff

Sig.ra Caterina Agnello
cagnello@unime.it

**UNITA' OPERATIVA PROGRAMMI DI RICERCA
INTERNAZIONALE**

Responsabile

Dr.ssa Francesca Pollicino
francesca.pollicino@unime.it – 090 676 8533

Vice Responsabile

Dr. Letterio Sacca
letterio.sacca@unime.it – 090 676 8572

D. A. Ricerca Scientifica e Internazionalizzazione

Dr.ssa Barbara Cafiso
barbara.cafiso@unime.it – 090 6768283

DOTTORATO DI RICERCA IN FISICA

*Dipartimento di Scienze Matematiche e Informatiche,
Scienze Fisiche e Scienze della Terra (MIFT)*
UNIVERSITÀ DEGLI STUDI DI MESSINA



**V.le F. Stagno D'Alcontres
S. Agata, Messina, Italy
e-mail: vcrupi@unime.it
ISSN: 2038-5889**