



# Appunti di Fisica '17 & Dottorato di Ricerca in Fisica

**21 dicembre ore 15:00**  
**Sala seminari, CNR-IPCFCN**

## **Protein Dynamics and Allosteric Properties in the Terahertz Regime**

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Allostery is defined as any process in which an event at one site of a protein (e.g. the binding of a ligand) impacts the structure and or dynamics of another site, thereby affecting its binding affinity towards a specific ligand and as a consequence modulating the protein activity. Such a process involves a long-range communication between the two sites that can be mediated both by changes in structure and in dynamics.

Over recent years the role of protein dynamics in allostery has been widely investigated in the picosecond-to-millisecond time scale, while the potential relation of faster intramolecular vibrations in the terahertz (THz) frequency range to allosteric effects is almost unexplored. Recently, the importance of these fast fluctuations has become a topic of intense debate for several processes occurring in biomolecules, e.g. in mediating efficient protein-ligand binding and in initiating and modulating slower dynamical processes. In the framework of molecular recognition, shedding light on the role of the THz dynamics of proteins could provide significant insights into the fine determinants of dynamic allostery.

In this contribution, we present a molecular dynamics simulations study of two model PDZ domains with differential allosteric responses. By characterizing the dynamic modulation of the protein induced by ligand binding, and focusing on the THz frequencies as opposed to a lower frequency regime, we identify a response nucleus that is visible only in the THz regime. The overlap between the known allosterically responding residues of the investigated PDZ domains and the response nucleus highlighted here suggests that fast THz dynamics could play a role in allosteric mechanisms.

The characterization of the THz dynamics by means of the proposed computational approach might provide a robust basis for the interpretation of the experimental results obtained with the emerging THz spectroscopy techniques.

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