DIPARTIMENTO DI SCIENZE MATEMATICHE E INFORMATICHE, SCIENZE FISICHE E SCIENZE DELLA TERRA
Dottorato di Ricerca in Fisica

Appunti di Fisica '24

11 aprile ore 15:00
Sala Seminari, CNR-IPCF

Prebiotic chemistry from ab initio & machine learning calculations

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In exploring the origins of life, the combination of *ab initio* calculations and machine learning is unlocking new insights. This research focuses on how glycine, a simple yet essential amino acid, can form through processes not previously identified. By using quantum simulations and advanced sampling methods, we've found a new pathway for glycine creation, the 'oxyglycolate path,' which might better explain its presence in meteorites. This method steps away from the traditional and more complex Strecker synthesis, suggesting simpler origins of life's building blocks. Machine learning is key here, as it helps us manage the heavy computational load, making it easier and more efficient to explore various chemical possibilities. This mix of high-level calculations and smart algorithms not only makes our research more effective but also opens the door to discovering previously unknown chemical reactions that could have led to life. Our findings not only challenge the old theories but also pave the way for new research into the chemical beginnings of life, all while making the process less intimidating and more accessible.