Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad - 500107

Seminar

Molecular Design using Traditional Computations and Machine Learning

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One of the principal outcomes of computations and experiments alike in chemistry is the ability to design and realize hitherto unknown molecules with desirable properties. Conventionally, computational methods such as quantum mechanical and density functional theory are systematically employed to understand the underlying factors responsible for a given phenomenon, which is then utilized to conceive new molecules to improve predictions. Alternatively, last few years have witnessed a surge in the use of modern machine learning methods for problems in chemistry and biology, which to some extent is changing the nature of computations that we are used to. The first part of the talk will discuss the results of a systematic exploration of the chemical space for identifying molecules with tetra coordinate-tetrahedral centers that can undergo racemization via a planar transition or intermediate state without having to break a covalent bond. The thermodynamic, kinetic and dynamic properties derived from state of the art computational methods that include high level ab initio calculations, Born-Oppenheimer molecular dynamics simulations and direct chemical dynamics simulations will be presented. In the second part of the talk, we will discuss the use of modern machine learning generative methods such as reinforcement learning and variational encoders for de novo molecular design. The ability of these methods to predict molecular structures starting from molecular properties instead of the conventional molecule to property prediction will be discussed. Case studies involving generation of small organic and inorganic molecular structures with desired properties such as molecular volume, logP and formation enthalpy will be presented.

Thursday, Nov 7th 2019

4:00 PM (Tea/Coffee at 3:30 PM)

Auditorium, TIFR-H