Tata Institute of Fundamental Research
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Internal Webinar

High-throughput exploration of materials with ab-initio methods

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Crystal Structure Prediction has remained an open problem in materials science. For a given composition, a method for predicting the most stable structure has not been devised. Some efforts have been made to classify elemental and binary solids through Pettifor structure maps, which generally identify stable structures of compounds that exist in highly symmetric chemical environments. In the first half of the presentation, chemical environments of 4 non-trivial space groups will be discussed. A systematic construction of a new dataset of materials reveals trends in stabilities of systems. Group-subgroup relationships of the chosen materials reveals how new stable materials can be found without a large sampling. The importance of electronic structure of a system is also emphasised when total density of, states is used as a descriptor for classifying different space groups.

Although the 3D materials are studied much more widely than compared to their lower dimensional counterparts, constructing structure maps and understanding model phenomenological effects becomes difficult. The second half of the presentation focuses on discussing 1D polymers that are reminiscent of the structure of ferrocene. Combining a hetero-substituted ring with a copper atom with the 7 possible frieze groups creates a database of new polymers. Structure-property relationships are established and comments about how these structures are interconnected in the potential energy surface are made. Modifications are made to the Coulomb matrix descriptor to satisfy the requirement of a periodic system. A one to one mapping is established with the components of the new descriptor and their contribution to the cohesive energy of a system.

All the computed data will be available for open access on MolDis, our Big Data analytics platform.

Monday, Jun 15th 2020

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