Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Internal Webinar

Fitting the potential energy surfaces using two layer networks and going up to deep learning architecture

Shweta Jindal

Academia Sinica, Taiwan

Exploring the structure and properties of metallic nanoparticles and molecular clusters with accuracy of the ab initio methods is a resource intensive task due to the increasing cost of the ab initio methods and number of distinct conformers as size increases. To counteract on this problem, we will use neural networks to fit the potential energy surfaces of metallic nanoparticles and molecular clusters. Neural networks provides a solution to bridge the gap between accuracy of ab initio methods and low computational costs. The accuracy of neural networks can be improved when the layers are increased.

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10:30 AM