Network for Computational Nanotechnology
Seminar Series

PURDUE UNIVERSITY Discovery Park

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Tuesday, November 8th 10:30am-12pm
Birck Nanotechnology Center, Room 1001

Machine learned approximations to Density Functional Theory Hamiltonians - towards high-throughput screening of electronic structure and transport in materials

Industrial applications often require high-throughput screening of the electronic structure of material systems for variations in system size, boundary conditions, geometry and strain. It is well known that DFT electronic structure and transport calculations scale poorly with system size. Even the so-called Order(N) DFT approaches do not scale to the extent required for time-sensitive electronic structure screening applications.

We present results from our recent work on direct machine learning of DFT Hamiltonians. We show that approximating DFT Hamiltonians accurately by direct learning is feasible and compare them to existing semi-empirical approaches to the problem.

The technique we have proposed requires little manual intervention or arbitrary model parameters and can be applied to any material system or geometry for quick-yet-accurate predictions of DFT Hamiltonians. We also discuss open questions and challenges that need to be addressed to integrate this technique into existing genomic approaches to materials discovery.

Ganesh Hegde is a Senior Research Scientist in the Advanced Logic Lab at Samsung Semiconductor Inc. His research involves the creation and use of advanced electronic and atomic structure approaches to describe and predict properties of materials relevant to logic technology. He is an author of 15 peer reviewed publications and an inventor on 10 US Patents and/or patent applications. He has a PhD in Electrical Engineering from Purdue University.