Framework for Coupling Machine Learning and *Ab Initio* Approaches

Scientific Achievement

Developed a computational framework for using neural networks to learn analytical potentials, non-linear density functionals, and structure-property relationships based on high-accuracy *ab initio* data. Demonstrated the use of neural networks to create easily evaluated local DFT charge-density functionals for a range of properties, including kinetic energy, correlation energy (at the CCSD(T) level), and bandgap (at the GW level) for a model gas-phase system, NH_3.

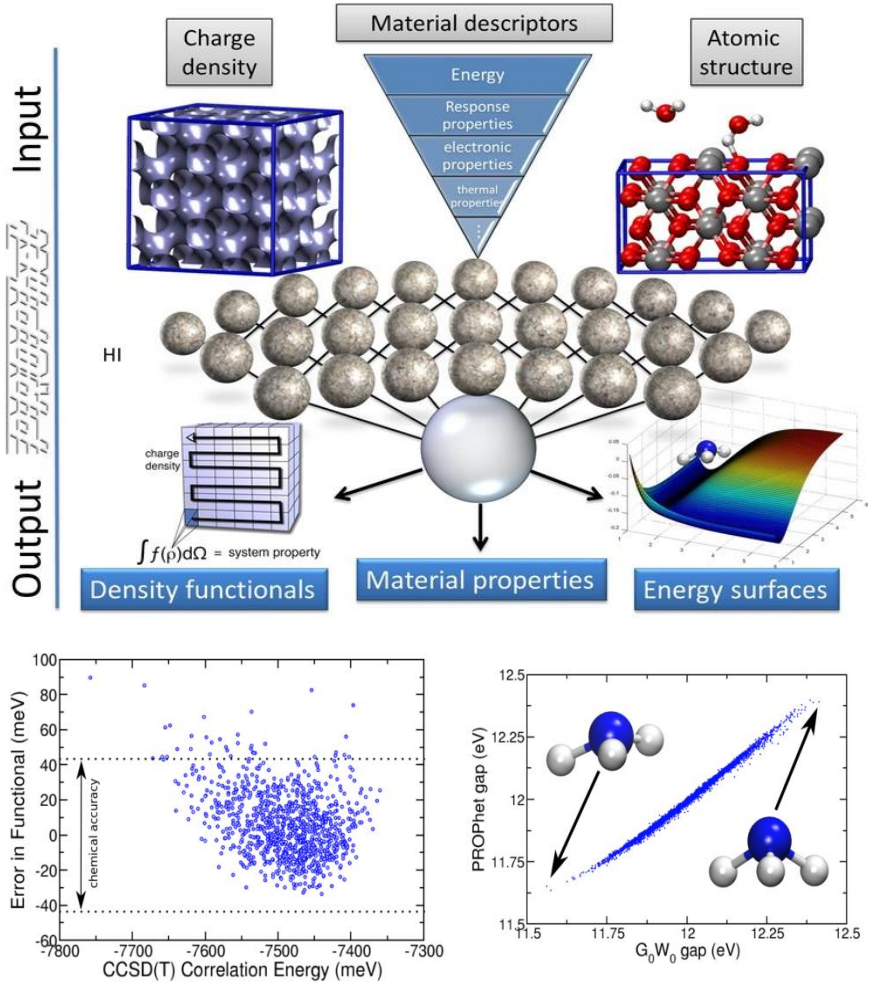
Significance and Impact

Developed PROPHet, an open-source code for coupling neural-network machine learning and first-principles methods. These tools enable new approaches for highly accurate mesoscopic simulations, rapid and accurate computation of otherwise expensive properties, and development of fundamental predictive models.

Research Details

- First code for analytical neural-network potentials directly integrated with the LAMMPS MD code.
- Enables use of grid-based data (i.e., charge densities) as input into neural networks.
- Open-source code (kolpak.mit.edu/PROPhet).

B. Kolb, L.C. Lentz, A.M. Kolpak, *Sci. Rep*. **7**, 1192 (2017).



Top: Overview of PROPhet. *Bottom:* Prediction of correlation energy (left) and bandgap (right) using neural-network learned charge-density functionals.

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