



# QMC-HAMM: From accurate correlated quantum simulations to mesoscopic scales

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**ENERGY**

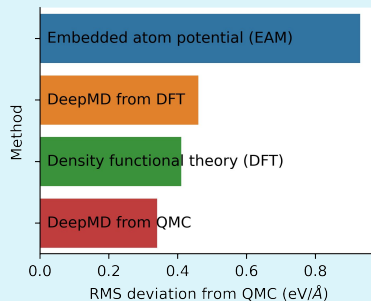
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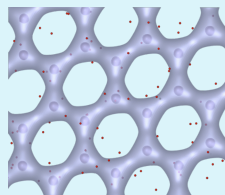
## The necessity of higher accuracy first principles data for multiscale modeling



Modern machine learned potentials (ML-DFT) are similar in accuracy to density functional theory (DFT).

Calculations for hydrogen at high pressure.

## Our strategy to deliver accurate models based on quantum Monte Carlo



A QMC sample of graphene. Each red dot is one electron.

Explicit correlation  $\rightarrow$  higher accuracy

**Data products:** QMC calculations are curated and published so others can use the high accuracy data.

**Software products:** Workflows and glue code to match QMC results to larger length scales.

Accuracy  $\Delta$

### Quantum Monte Carlo

- Explicit correlation
- High accuracy
- Large computational cost

### Density Functional Theory

- Implicit correlation
- Lower accuracy
- Lower cost

### QMC-ML models

- Quantum lattice models (tight binding)
- Atomistic potentials

### DFT-ML

- Quantum lattice models (tight binding)
- Atomistic potentials

### QMC-HAMM approach

### QMC Mesoscale

- Phase diagrams
- Continuum models
- $k \cdot p$  models

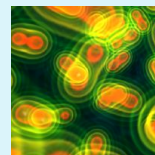
### DFT mesoscale

- Phase diagrams
- Continuum models
- $k \cdot p$  models

Standard approach

Maximum time/length scales  $\triangleright$

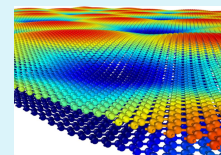
## High pressure hydrogen



A QMC **data set** (energies and forces on protons) is prepared for hydrogen at high temperature and pressure.

The model is used to compute the melting line of hydrogen. See **QMC-HAMM P1**

## Twisted bilayer graphene



A highly accurate local environment tight-binding model LETB for twisted bilayer graphene. **QMC-HAMM P2**

The interaction potential between layers. **QMC-HAMM P3**

Computing effective interactions at the Moire' scale. **QMC-HAMM P4**