qmc-hamm.github.io

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

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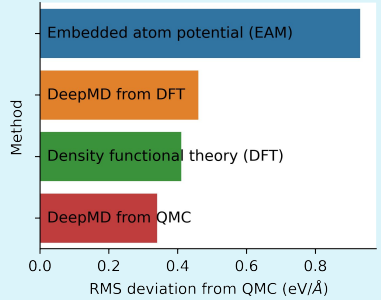
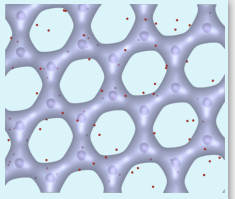


The necessity of higher accuracy first principles data for multiscale modeling

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

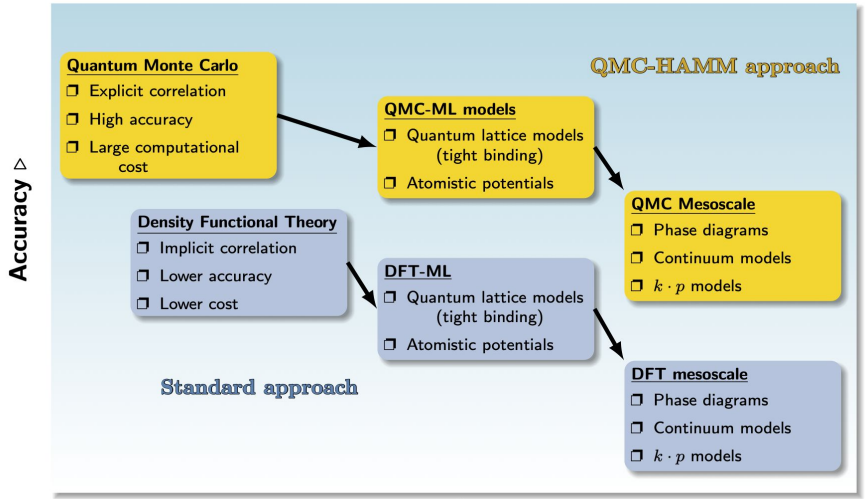


A QMC sample sample on graphene. Each red dot is one electron.

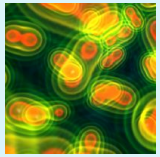
Explicit correlation -> higher accuracy

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.



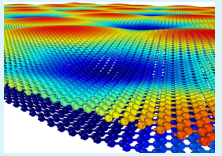
High pressure hydrogen



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