Graphene-Water Non-Bonded Interaction from First Principles
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Control Water at Nanoscale

Nanoscale water interfaces

Manipulating trapped water using STM tip: Reduce water layer thickness locally by applying a voltage bias (He et al. Nano Lett. 2012)

Fast water rotation inside C₆₀ (Kurotobi and Murata, Science 2011)

Fast water transport in carbon nanotube (Hall et al. Science 2006)

We’d like to have control of these interfaces for design in applications like desalination, sensing, nanomanufacturing, etc.

Solve Many-body Schrödinger Equation

Target $H_V(X) = E_{X}(X)$

Solve a different equation in Diffusion Monte Carlo (DMC) method

Isomorphism between Schrödinger equation and stochastic process

Wavefunction ↔ Distribution of walkers

Kinetic ↔ Diffusion

Potential ↔ birth/death

Verify and calibrate DMC method

Example: harmonic oscillator

Graphene-Water Interaction is Strong

The binding energy is 180±20 meV.

The binding energy has a weak water-orientation dependence.

Insights by Comparing with Experiments

Experiment set (for single water)

Heat of adsorption of a single water molecule on graphite

Heat of adsorption energy of water on graphite from gas chromatograms, extrapolated to zero water density (Kiselev et al. 1969)

Our calculation agrees with experiments involving a single water molecule.

Graphene-water interaction is not additive. Why?

We Don’t Know How Water Interacts with Carbon

Change in carbon-water interactions leads to different properties

Water contact angle on graphene

CNT filling behavior

Fast water transport through CNT

Determining carbon-water interaction from experiments is challenging

Change in water contact angle on graphene with time when exposed to air (Li et al. Nature Material 2013)

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Single Water has Charge Transfer while Liquid Water doesn’t

Charge transfer by looking at energy levels

Charge transfer observed for single water from our electron density analysis!!!

Electron density redistribution when a single water molecule approaches graphene.

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