First-Principles Molecular Dynamics

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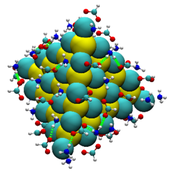
Qbox
First-Principles Molecular Dynamics

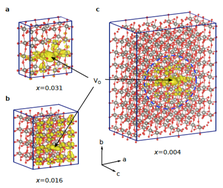
- C++/MPI/OpenMP implementation of FPMD
- Large-scale parallelism (used on up to 128k cores on ANL Mira)
- New developments
  - Implementation of the SCAN meta-GGA functional
  - Implementation of RSH (range-separated hybrid), DDH (dielectric dependend hybrid), HSE (Heyd-Scuseria-Ernzerhof) hybrid functionals
- Integration of recent developments
  - Response to arbitrary external fields
  - Polarizability

First-Principles MD Applications

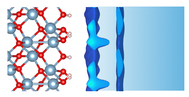


Stability of CdSe nanoparticles in contact with organic ligands

Polaron formation in non-stoichiometric WO_3



M. Gerosa, F. Gygi, M. Govoni, G. Galli, *Nature Materials* (2018) (in press)

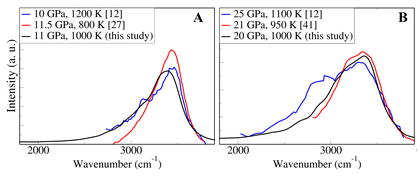


Structure of the Al_2O_3/H_2O interface

Spectroscopy Applications

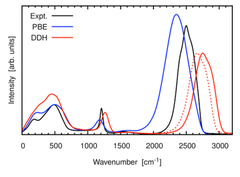
- Raman spectroscopy from FPMD simulations including calculations of polarizability
- IR Spectroscopy from FPMD simulations using on-the-fly calculations of the polarization

Raman spectrum of water at high pressure



V. Rozsa, D. Pan, F. Giberti, G. Galli, *PNAS, 201800123* (2018)

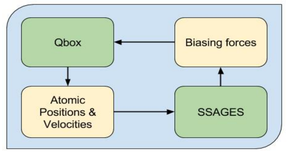
Infrared spectrum of water computed using a delectric-dependent hybrid functional (DDH)



A. Gaiduk, J. Gustafson, F. Gygi, and G. Galli, *J. Phys. Chem. Lett.*, 9 3068 (2018)

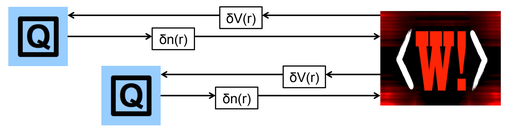
Client-Server Operation

- Qbox can be used by other codes as a "DFT-engine"
  - Generates DFT/hybrid-DFT energies and forces
  - Generates density response to arbitrary external potentials
- Communication implemented through the file system
- Qbox-SSAGES coupling
  - Free energy calculations using PBE and PBE0 energies and forces



E. Sevgen, F. Giberti, H. Sidky, J.K. Whitmer, G. Galli, F. Gygi, J.J. de Pablo, *JCTC* **14**, 2881 (2018).

- Qbox-WEST coupling
  - Calculation of the dielectric response used in GW and BSE approximations
  - Multiple Qbox instances running in parallel



Infrastructure

Software distribution

- Qbox web site http://www.qboxcode.org
- Qbox GitLab server http://scherzo.ucdavis.edu/qbox/qbox-public
- GitHub mirror https://github.com/qboxcode
- Online Documentation using Sphinx-doc
- Tutorials/Examples development
- Analysis tools

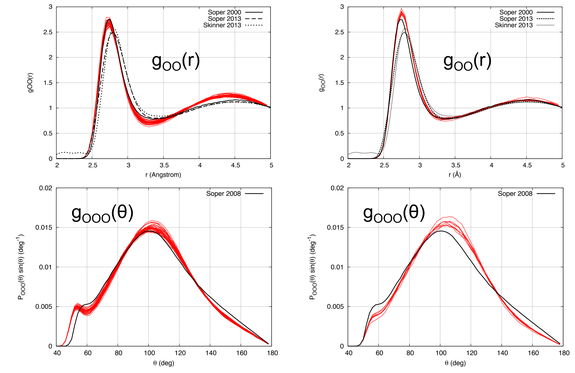
Pseudopotentials

- SG15 collection based on Hamann ONCV formulation
- M. Schlipf, F. Gygi, Comput. Phys. Comm. **196**, 36 (2015)
- Ongoing validation of all elements (from H to Bi)
- Curation of the SG15 pseudopotential collection at http://quantum-simulation.org
- Potentials distributed in Qbox and UPF (QE) formats
- Validation of the use of PBE pseudopotentials with hybrid-DFTs

DFT MD Reference Datasets

- The availability of reference datasets allows for quantitative comparisons of density functionals
- Focus on H_2O, relevant to several applications
- PBE400 Dataset
  - 32-sample ensemble simulations, PBE, *T*=400 K
    - W. Dawson, F. Gygi, J. Chem. Phys. 148, 124501 (2018)
- SCAN330 Dataset
  - Perdew's SCAN meta-GGA functional (Sun et al. PRL 2015)
  - Shown to improve agreement with experiment w.r.t. PBE
  - 8 independent samples, 45 ps each, *T*=330 K
    - M. LaCount, F. Gygi (in preparation)
- Full data available online (including trajectories)
  - http://www.quantum-simulation.org/reference

PBE400 SCAN330



Pair correlation functions ($g_{OO}(r)$) and angular correlation functions ($g_{OOO}(\theta)$) of ensemble simulations enable quantitative comparisons of density functionals

Future Directions

- Platform-independent performance
  - Autotuning kernels
- Streamlining spectroscopy applications
  - Beyond IR or Raman simulations
- Coupling through wave function sharing
- Dynamic loading of custom plug-ins
  - Let users define their own Qbox command
  - Facilitate development/extension by new users

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