BEAST: Beyond-DFT Electrochemistry with Accelerated and Solvated Techniques

The BEAST collaboration

1st Annual BEAST Workshop, 2022
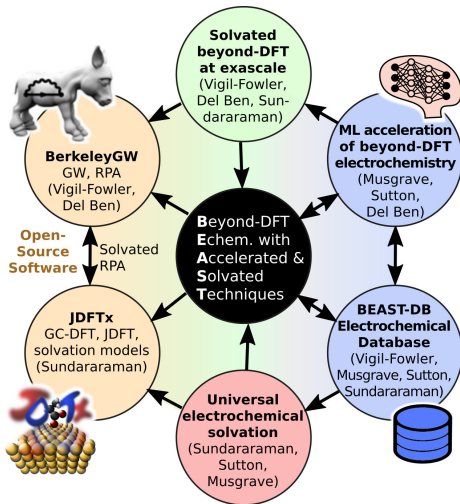
August 15, 2022

The BEAST project

Goals:

- ▶ Universal solvation using joint density-functional theory (JDFT)
- ▶ Solvated electrochemical RPA calculations with exascale codes
- ▶ Machine-learned acceleration for rapid RPA-quality predictions

PI Team:

- ▶ R. Sundararaman (RPI)
- ▶ D. Vigil-Fowler (NREL)
- ▶ C. Musgrave (CU Boulder)
- ▶ C. Sutton (U South Carolina)
- ▶ M. Del Ben (LBNL)

The Need for BEAST

First-principles for electrochemistry typically:

- ▶ Ignore electrolyte entirely, or use overly simplistic implicit models, and
- ▶ Use DFT, which can be inaccurate for electronic structure of interfaces.

To address, this BEAST aims to:

- ▶ Make accurate solvation methods readily available to the electrochemistry community, and
- ▶ Couple them with many-body methods such as RPA for accuracy beyond the DFT level.

Review article from the BEAST team:

R. Sundararaman, D. Vigil-Fowler and K. Schwarz,
'Improving the Accuracy of Atomistic Simulations
of the Electrochemical Interface,'
Chem. Rev. **122**, 10651 (2022)

BEAST software: JDFTx and BerkeleyGW
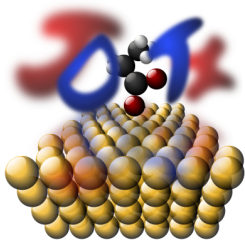
- JDFTx: plane-wave electronic DFT in:
    - Vacuum
    - Polarizable continua
    - Classical density functional fluids
- Grand canonical calculations for electrochemistry
- Algebraic formulation for rapid theory development

BEAST software: JDFTx and BerkeleyGW

http://jdftx.org
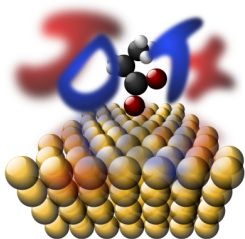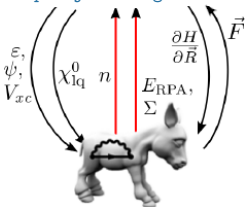

https://berkeleygw.org

- ▶ JDFTx: plane-wave electronic DFT in:
  - ▶ Vacuum
  - ▶ Polarizable continua
  - ▶ Classical density functional fluids
- ▶ Grand canonical calculations for electrochemistry
- ▶ Algebraic formulation for rapid theory development
- ▶ *Coming soon*: solvated GW and RPA via BerkeleyGW as a part of the BEAST project

Annual BEAST workshops

Goals:

- ▶ Train computational electrochemists in state-of-the-art solvated electronic structure methods
- ▶ Feature recent methodological developments in the related software projects

New features planned to be introduced at each workshop:

1. Online workshop 2022: JDFTx – BerkeleyGW interface
2. In-person workshop 2023: Solvated RPA calculations
3. Online workshop 2024: BEAST-DB usage and classical DFT solvation
4. In-person workshop 2025: combined functionality of all the above