BEAST: Beyond-DFT Electrochemistry with Accelerated and Solvated Techniques

The BEAST collaboration

3rd Annual BEAST Workshop, 2024

August 22, 2024

U.S. DEPARTMENT OF ENERGY

Office of Science

Award # DE-SC0022247

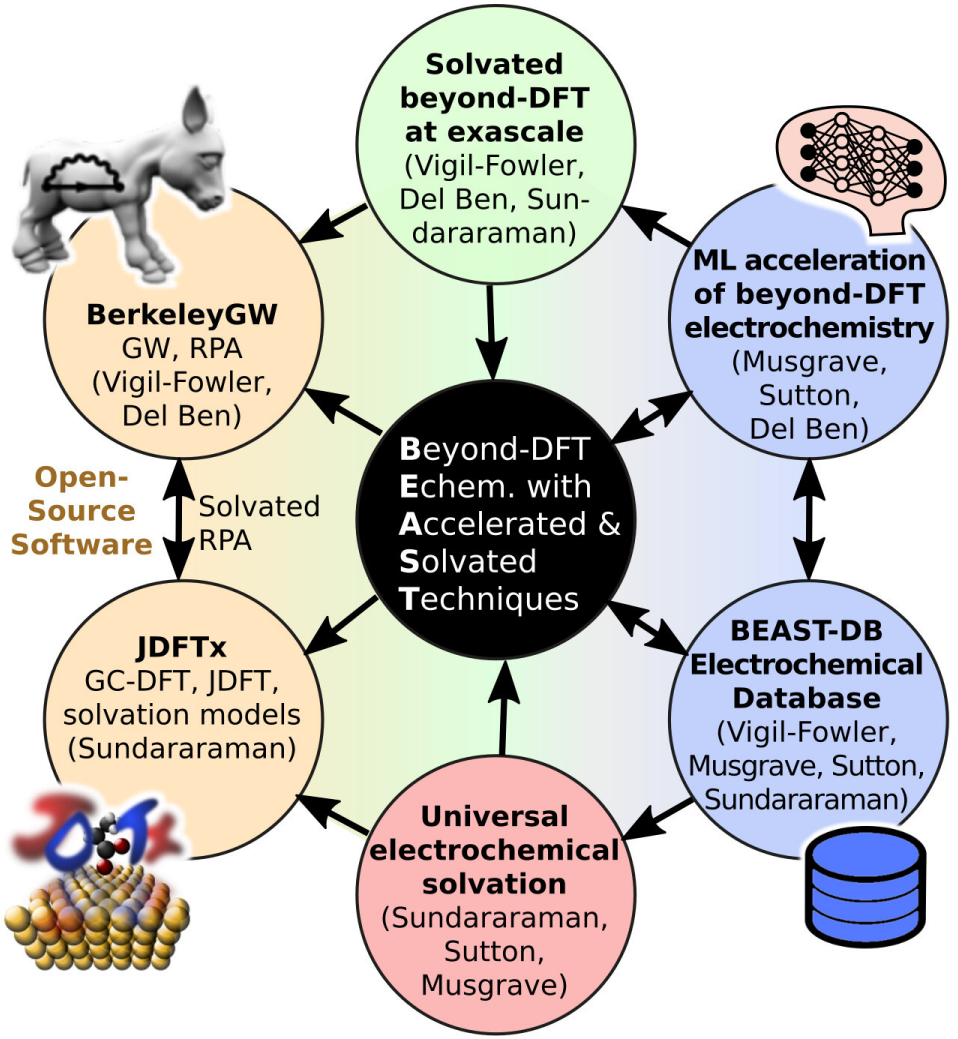
The BEAST project

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)



Rensselaer NREL South Carolina BERKELEY LAB

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.

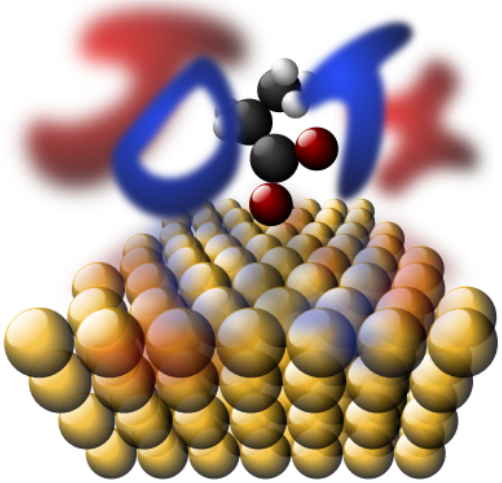
To address, this BEAST aims to:

- 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



http://jdftx.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

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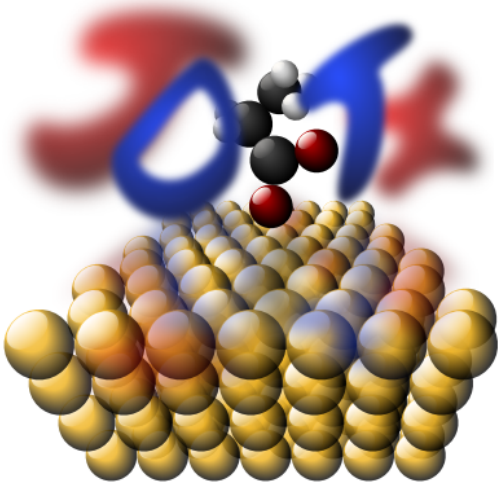

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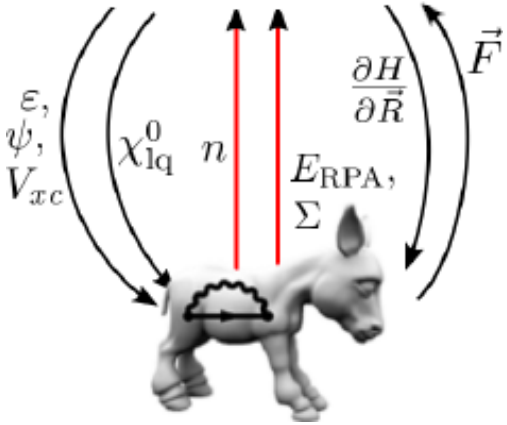

https://berkeleygw.org

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  - Classical density functional fluids
- Grand canonical calculations for electrochemistry
- Algebraic formulation for rapid theory development
- *NEW*: solvated GW via BerkeleyGW as a part of the BEAST project
- *NEW*: BEAST-DB database with GC-DFT calculations
- *Coming soon*: QimPy code for further scaling electrochemistry calculations

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 GW calculations and QimPy preview
3. In-person workshop 2024: BEAST-DB usage and RPA calculations
4. In-person workshop 2025: combined functionality of all the above