LA-UR-18-27667

Approved for public release; distribution is unlimited.

Title:	Modeling solid-liquid interfaces using next generation quantum molecular dynamics
Author(s):	Kleiner, Kevin Gordon Nair-Kanneganti, Aparna Gonzales, Ivana Negre, Christian Francisco Andres Niklasson, Anders Mauritz
Intended for:	XCP CPSSW 2018 Quick Look and Final Poster Presentation
Issued:	2018-08-10

Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Modeling solid-liquid interfaces using next generation quantum molecular dynamics

Self-consistent charge convergence

Aparna Nair-Kanneganti and Kevin Kleiner
Mentors: Christian Negre, Ivana Gonzales,
and Anders Niklasson

August 13, 2018

Kevin Kleiner

- Rising senior at the University of Tennessee Knoxville: physics major and math minor
- Research interests: computational atomic scale many-body simulations/calculations
- Background: computational condensed matter physics with classical Monte Carlo simulations of crystal lattices and a little machine learning with neural networks
- Undergraduate physics teaching assistant and tutoring experience

Aparna Nair-Kanneganti

- Rising junior at Yale University, majoring in Applied Physics with a concentration in quantum computing
- Formerly of the Reeke Group at the Rockefeller University in New York, and the Brown Group at Yale University
- Research interests span physics and computational science: hierarchical space partitioning algorithms, MHD phenomena, micromechanical oscillators

Catalyzing Fuel Cell Reactions

Fuel cell schematic

Cathode atomic setup

Investigating Catalytic System Electron Transfer

- DFTB (density functional tight binding theory) is a descendant of DFT
- Equations of motion from extended Lagrangian with charge density constraint
- Initial self-consistent charge density $\rho[n]$ obtained by solving nonlinear eigenvalue problem

$$H[n]\psi_i = \epsilon_i\psi_i, \rho[n] = \sum_{i \in occ} |\psi_i|^2$$

Initial Charge Convergence Data

Charge residual convergence for graphene

Charge residual convergence for graphene with O_2 and H_2O