Introduction

Molecular simulation and quantum chemistry software is an integral part of chemistry and biology, and has been broadly adopted by academic researchers and industry scientists. These advances in simulation software will be enabled by the deployment of state-of-the-art theoretical models and algorithms that are developed to tackle the grand challenge problems of computational chemistry and biology. For example, recent advances in approximate polarizable models and algorithms that can mitigate the cost, implemented on high performance computing platforms, will be enabled by the deployment of state-of-the-art theoretical models and industry scientists. Next generation scientific breakthroughs that utilize chemical and biological applications, first development, electronic structure methods, new state-of-the-art codes and highly developed open-source libraries, to directly tackle these obstacles. Our US and UK collaboration between silicon and classical chemistry, making possible the development of advanced potential energy surface models, successfully deployed on current and next generation high performance computing platforms.

Advanced Potential Energy Surfaces

The instantaneous physical state of a molecule is determined by its potential energy surface (PES). The PES is a function of the coordinates of all the constituent atoms, and includes contributions from the electronic structure, nuclear repulsion, and interatomic interactions. The PES can be expressed as

\[ U(r) = U_e + U_{el} + U_{int} \]

where \( U_e \) is the electronic energy, \( U_{el} \) is the electrostatic energy, and \( U_{int} \) is the interatomic energy. The PES is often approximated by a polynomial function of the coordinates, known as a potential energy surface model.

Small scale problems and full couplings are being routinely tackled by ReadyTalk and Zoom, and is also covered by a Giroard account at the University of New York.

We would like to thank the Natural Sciences Foundation (NSF-CHE-1265731; NSF-CHE-1265889; NSF-CHE-1265704; NSF-CHE-1453123) and the Engineering and Physical Sciences Research Council (EPSRC-EP/N023939/1) for supporting this work.

Polaronization Applications

Our consortium is organized in part around the classical force field AMOEBA (Atomic Multipole Embedded Optimized Boundary Approximation) approach to electronic structure calculations. AMOEBA is a hybrid quantum mechanical/molecular mechanical force field, where the electronic structure calculations are performed using the QM/MM method, and the quantum mechanical wavefunction is approximated by a polarizable force field. AMOEBA is implemented in the ONETEP and Q-MOM software packages, which are designed to handle large-scale calculations.

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We completed the second year of our molecular simulation bookshop last June that took place June 19-21, 2015. The bookshop featured a series of lectures on advanced computational techniques, with special emphasis on the development of state-of-the-art force fields for applications in chemistry and biology.

A Workshop titled June 15-19, "Development and deployment of advanced chemical software for potential energy surface surfaces" attended by all US-UK participants.

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