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Editorial

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Beyond QM/MM: Fragment Quantum Mechanical Methods

The idea of developing a Special Issue on "Beyond QM/MM: Fragment Quantum Mechanical Methods" for macromolecular simulations was conceived in March 2013 at Mesilla, New Mexico, where the Senior Editor (K.N.H.) and one of the guest editors (J.G.) attended the annual Mesilla Workshop on chemical dynamics. This proposal was warmly supported by the Editors, and an issue was quickly slated to be published in 2014. A few months later, we learned that the 2013 Nobel Prize in Chemistry was awarded to Martin Karplus, Michael Levitt, and Arieh Warshel for their contributions to combined quantum mechanical and molecular mechanical (QM/MM) methods, a class of multiscale models, to study chemical and biological reactions. Now, we are delighted to have the opportunity to present this Special Issue to celebrate this great event in computational chemistry.

In the past 20 years, combined QM/MM methods have matured to become a method of choice for studying chemical processes in large systems. Parallel to this advance is the development of molecular mechanical force fields, particularly those used to model biological systems such as proteins and nucleic acids. However, there are also several well-known limitations that cannot be resolved within the framework of either MM or combined QM/MM. To further improve the accuracy of computational models in order to make quantitative prediction and interpretation of biomolecular interactions and materials design, there is a great need to go beyond the classical representation or mixed quantum and classical models.

Currently, we are witnessing a burst of exciting advancements that involve representing the entire biomolecular and condensed-phase systems directly using quantum chemical models. In principle, quantum mechanics can provide both reactive and nonreactive potential energy surfaces, in which electronic polarization, electron correlation, and charge transfer are naturally included. These methods, in one way or another, rely on the partition of a large system into molecular fragments such that the computational cost is reduced from a formally $O[(MN)^k]$ scaling to $O[(M \log M)N^k]$, where M is the number of fragments, N is roughly the number of electrons in one fragment, and k is the power law for the computational effort of the particular QM model used (e.g., $k = 3$ for matrix diagonalization, 4 for Hartree-Fock theory, 5 for second-order Møller-Plesset perturbation theory (MP2), and 7 for coupled cluster theory CCSD(T)). Fragment quantum mechanical methods can be used either as an electronic structure theory for macromolecules or as a quantum mechanical force field (QMFF). Both directions represent paradigm-shifting advances in the way that we represent and model biomolecular and condensed-phase systems. These methods have the potential to greatly increase the accuracy and predictability of computational models for chemical processes. The present Special Issue features a selection of 17 contributions from leading experts, covering a wide range of topics. We hope that this collection of papers will help further stimulate methods development and increase the scope of novel applications.

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