Improving the Accuracy of Quantum Chemistry Methods with Optimized Effective Potentials

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The perennial challenge in applied quantum chemistry is balancing the computational resources (time, disk, memory) associated with simulation work with the accuracy of the results obtained. Our recent efforts have focused on the development of a modification to approximate density-functional (DFT) and wavefunction theory methods to improve their accuracy to that associated with highly-correlated (and resource intensive) wavefunction theory and experimental results. Our approach, which can be described as a Δ-DFT (or Δ-machine learning) method, is based on optimized atom-centered potentials (ACPs). Unlike machine learning approaches, ACPs can be developed using datasets consisting of as few as 100 data points. The potentials are "shaped" such that they mitigate the errors associated with common computational chemistry methods, including incomplete wavefunction descriptions, poor DFT descriptions of exchange/correlation, delocalization error, and so on. The optimized ACPs are used in conjunction with the computational method for which they were developed and require little – if any - additional computing resources. The ACP concept, development process, their applications and performance will be presented.

Biography

Gino DiLabio is a full professor in the Department of Chemistry at The University of British Columbia's Okanagan campus, which he joined in 2014. In addition to methods development, his research interests include non-Aufbau behaviour in radical enzymes, radical chemistry in general, and electric field catalysis at water interfaces. Prior to joining UBC, he was a senior staff scientist at Canada's National Institute for Nanotechnology (now the Nanotechnology Research Centre) where he worked on the development of novel quantum cellular automata and hybrid organic-silicon systems. He has published more than 150 papers, patents, and book chapters.