

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Optimization of Ionization-potential Improved Range-separated Density Functional Theory¹ YIFAN JIN, RODNEY BARTLETT, University of Florida — The physical meaning of the Kohn-Sham eigenvalues is traditionally not quite clear. But it is essential for the density functional theory, which is usually designed empirically, to converge to the right answer. The currently developed range-separated density functional methods in the QTP family, that is, the CAM-QTP00 and CAM-QTP01, are designed to make the Kohn-Sham eigenvalues of all the occupied orbitals good approximation to the exact ionization energies. The benchmark calculations have shown that these methods, especially the CAM-QTP01, could improve the ionization and excitation energies along with the chemical and physical properties of the ground states. However, they still could not well reproduce certain properties such as the atomization energies of the large organic molecules. During the recent work, the methods were further optimized with larger training sets and new algorithm. And the accuracy of those ground and excited states properties was further improved. The basic principles, strategy of functional optimization and the benchmark results will be presented.

¹HPCMP Applications Software Initiative

Yifan Jin
University of Florida

Date submitted: 05 Jan 2017

Electronic form version 1.4