Generalized energy-based fragmentation approach for large molecules and condensed phase systems

Shuhua Li

School of Chemistry and Chemical Engineering, Institute of Theoretical and Computational Chemistry, Nanjing University, Nanjing, 210093, P. R. China
shuhua@nju.edu.cn

In this talk, I will report recent developments and applications of the generalized energy-based fragmentation approach (GEBF) developed by our group for large molecules and condensed phase systems. The GEBF approach is a linear scaling technique that allows ab initio ground-state calculations feasible to very large systems and condensed phase systems at ordinary workstations. Within this approach, the ground-state energy (or properties) of a large molecule can be evaluated directly from the corresponding quantities of various "electronically embedded" subsystems.[1] The GEBF approach has been established to be an efficient and reliable theoretical tool for investigating structures, relative stability, and properties of various complex systems.[2-5] With specifically designed fragmentation schemes, the GEBF approach can be extended to treat metal-containing large supramolecular coordination complexes and ionic-liquid systems.[6-7] The periodic version of the GEBF approach for systems with periodic boundary conditions (PBC-GEBF) has also been established.[8] The PBC-GEBF approach has been employed to obtain the optimized crystal structures and vibrational frequencies of molecular crystals.[9] Our applications demonstrate that the PBC-GEBF method, combined with advanced electronic structure methods, is capable of providing accurate descriptions on the lattice energies, structures, vibrational and NMR spectra for various types of molecular crystals.[10]

References

1. W. Li, S. Li, Y. Jiang, *J. Phys. Chem. A* **111** (2007), 2193.
2. S. Li, W. Li, J. Ma, *Acc. Chem. Res*. **47** (2014), 2712.
3. D. Yuan, X. Shen, W. Li, S. Li, *Phys. Chem. Chem. Phys.* **18** (2016), 16491.
4. D. Zhao, R. Song, W. Li , J. Ma , H. Dong and S. Li, *J. Chem. Theory Comput.* **13** (2017), 5231.
5. D. Yuan, Y. Li, Z. Ni, P. Pulay, W. Li and S. Li, *J. Chem. Theory Comput.* **13** (2017), 2696.
6. Y. Li, D. Yuan, Q. Wang, W. Li and S. Li, *Phys. Chem. Chem. Phys.* **20** (2018), 13547
7. D. Yuan, Y. Li, W. Li and S. Li, *Phys. Chem. Chem. Phys.* **20** (2018), 28894
8. T. Fang; W. Li; F. Gu; S. Li, *J. Chem. Theory Comput.* **11** (2015), 91
9. T. Fang, J. Jia, S. Li, *J. Phys. Chem. A* **120** (2016), 2700.
10. T. Fang, Y. Li, S. Li, *WIREs Comput. Mol. Sci* **7** (2017), e1297.