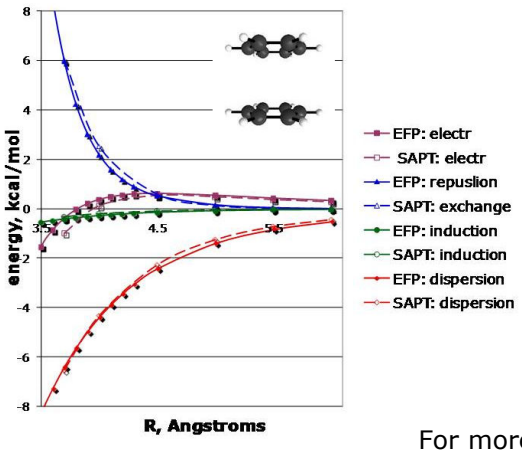
A Quantum Leap Into the Future of Chemistry

What's New in Q-Chem

Effective Fragment Potential (EFP) Method

Developers: Vitalii Vanovschii, Debashree Ghosh, Dmytro Kosenkov, Lyudmila Slipchenko, Anna Krylov

EFP is a model potential used to describe inter-molecular interactions in molecular clusters, liquids, and biologically relevant molecules like DNA bases. The cost of an EFP calculation is similar to that of force fields used in molecular mechanics, however, the EFP parameters are derived from the first principles and the mothod involves no empirical parameter fitting. EFP naturally provides the decomposition of the interaction energy in terms of Coulomb, polarization, dispersion, and exchange-repulsion components. EFP can be used for robust and predictive calculations of structures, binding, and interaction patters in weakly bound complexes and systems. For example, for different isomers of the benzene dimer, the largest discrepancy between EFP and CCSD(T)/CBS is 0.4 kcal/mol in binding energies and 0.2A in the equilibrium structures.



EFP and SAPT (symmetry-adapted perturbation theory) energy components for the sandwich configuration of the benzene dimer. An excellent agreement between EFP and SAPT demonstrates that the high accuracy of EFP is not due to error cancellation but is a result of accurate treatment of the physics of non-covalent interactions.

For more new features, visit:
www.q-chem.com/whatsNew4.html

The Design Center, Suite 690 • 5001 Baum Boulevard • Pittsburgh, Pennsylvania 15213 • United States of America
Telephone: (412) 687-0695 • Facsimile: (412) 687-0698 • E-Mail: info@q-chem.com
Website: http://www.q-chem.com

What's New in Q-Chem

Effective Fragment Potential (EFP) Method (continued)

Debashree Ghosh

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For more information on how to use this feature, refer to the Q-Chem Manual, Section :

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