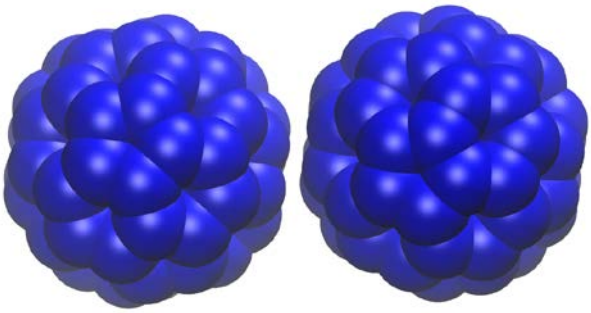
# Accurate Intermolecular Potential for the $C_{60}$ Dimer

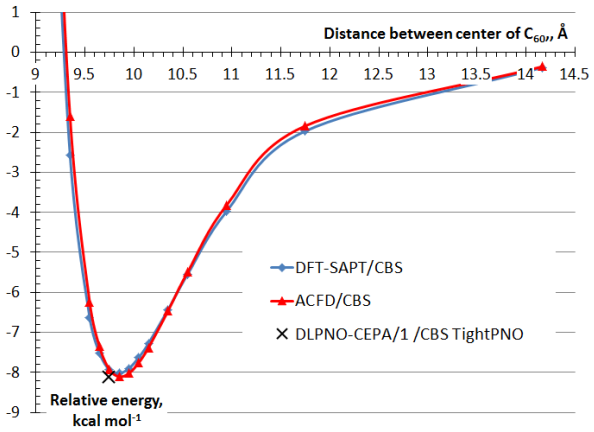
D.I. Sharapa[1], J. T. Margraf[2], A. Hesselmann[3] and T. Clark[1]

*[1] Computer-Chemie-Centrum, Department Chemie und Pharmazie, Friedrich-Alexander-Universitat Erlangen-Nurnberg,Nagelsbachstraße 25, 91052 Erlangen, Germany*

*[2] Quantum Theory Project, University of Florida, Gainesville, Florida 32611, United States*

*[3] Lehrstuhl für Physikalische und Theoretische Chemie, Friedrich-Alexander-Universitat Erlangen-Nurnberg, Egerlandstraße 3,91058 Erlangen, Germany*






The self-assembly of molecular building blocks is a promising route to low-cost nanoelectronic devices. It would be very appealing to use computer-aided design to identify suitable molecules. However, molecular self-assembly is guided by weak interactions, such as dispersion, which have long been notoriously difficult to describe with quantum chemical methods. In recent years, several viable techniques have emerged, ranging from empirical dispersion corrections for DFT to fast perturbation and coupled-cluster theories. We test these methods for the dimer of the prototypical building block for nanoelectronics, $C_{60}$-fullerene.

Benchmark quality data is obtained from DFT-based symmetryadapted perturbation theory (SAPT), the adiabatic-connection fluctuation dissipation (ACFD) theorem using an adiabatic LDA kernel, and domain-based local pair natural orbital (DLPNO) coupled-pair and coupled-cluster methods. These benchmarks are used to evaluate economical dispersion-corrected DFT methods, double-hybrid DFT functionals, and second-order Møller−Plesset theory. Furthermore, we provide analytical fits to the benchmark interaction curves, which can be used for a coarse-grain description of fullerene self-assembly. These analytical expressions differ significantly from those reported previously based on bulk data.[1]

[1] D.I. Sharapa, J. T. Margraf, A. Hesselmann and T. Clark, *JCTC*, **2017**, *13*, 274-285.