ACS

View Abstract

ABSTRACT SYMPOSIUM NAME: Quantum Mechanics

ABSTRACT SYMPOSIUM PROGRAM AREA NAME: COMP

CONTROL ID: 3658052

PRESENTATION TYPE: Oral Only : Consider for Sci-Mix

TITLE: Dispersion Size-Consistency within the Adiabatic Connection Symmetry-Adapted Perturbation Theory

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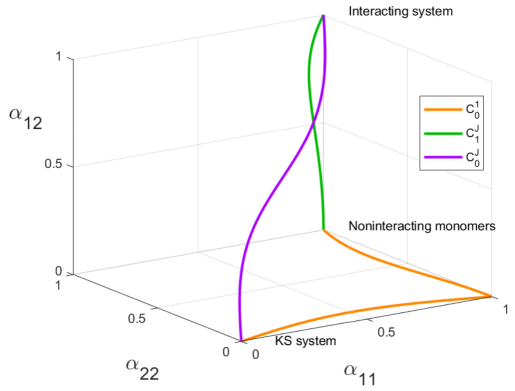
ABSTRACT BODY:

Abstract: Noncovalent interactions (NIs) play an important role in molecular biology, supramolecular chemistry, materials, and molecular crystals. The characterization and interpretation of NIs have remained a great challenge for experimentalists and theorists. In a previous work, Nguyen and coworkers [Nguyen, B. D. et al J. Chem. Theory Comput. 2020, 16 (4), 2258–2273.] developed the adiabatic connection symmetry-adapted perturbation theory (AC-SAPT) for nondegenerate dimers and established the importance of electrodynamic screening to understand NIs. The AC-SAPT series within the many-body perturbation theory (MBPT) spuriously diverges while AC-SAPT series within random phase approximation is always convergent. As follow-up to the previous work, I present an extension of the AC-SAPT formalism within dimers to N-monomers and establish the dispersion size-consistency condition which states that the total dispersion energy of a N-monomer system is independent of any partitioning into subsystem. The development of dipsersion size-consistency provides an additional condition to the Casimir-Polder size-consistency, which is evident in long-range dispersion interactions. Next, I explore disperion theories such as RPA, MBPT, and SAPT and determine which ones satisfy the dispersion size-consistency. Finally, dispersion energy calculations for RPA and MBPT are shown along with conclusions for electronic structure theory of NIs and future directions of modeling NIs.



The full interaction between two monomers is illustrated by the decomposition of the interaction path into the intermonomer interaction (α_{12}) and the intramonomer interactions (α_{11} and α_{22}).