Fourier representation methods for Møller-Plesset perturbation theory in one-dimensionally periodic systems

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Interpretation and prediction of the structural and electronic properties of polymers are often based on model systems with periodicity in one dimension. The currently most popular method for purely theoretical calculations of the electronic structure of extended systems is density functional theory (DFT). However, DFT includes electron correlation approximately and because most current functionals are not always adequate, a number of properties (band gap, ionization potentials, intermolecular interactions, ...) are not properly described. Accordingly, methodologies based on the Hartree-Fock theory and beyond retain their interest and obtaining suitable methods towards reliable and efficient computer codes should be continued.

A major challenge in electronic structure calculations of extended systems is to carry out to convergence the various (coulombic, exchange, ...) lattice sums. Convergence characteristics of the various lattice sums are now well established for the direct space formalism of the restricted Hartree-Fock (RHF) and MP2 equations.

This poster describes the use of the Fourier representation method, originally proposed by Harris and Monkhorst[1] and developed specifically by I. Flamand and the present authors[2] for systems periodic in one dimension, in ab initio studies that include many-body computation of electron correlation effects[3]. Second-order corrections to the restricted Hartree-Fock energy and energy band gaps are computed in the Møller Plesset scheme.

Systems investigated include H_2, Be and LiH chains and comparison is made with direct-space extended system and oligomer computations. The results confirm the validity of the methods and illustrate the improvement in convergence relative to direct-space computations.

References :
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