Stability and equilibrium structure


Due to its accurate account of both short-range and long-range (dispersive) interactions, LMP2 is particularly well suited for describing molecular crystals.

吸附 at crystalline surfaces


Using a slab supercell 2x2 model, He/MgO adsorption is well described by LMP2 while DFT performs unsatisfactorily.

One-electron Properties


The comparison of directional CPs of Si measured at SPring8 with calculated ones reveals definite inadequacies of the most popular theoretical models for the description of the EMD in crystals. LMP2 results are instead in good agreement with the experiment.

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Compton Profile Anisotropy in Silicon: $J_{[110]}(p) - J_{[100]}(p)$ (All data in a.u.)

… one step into electron correlation in crystals
Momentum Density (EMD), Compton Profiles, X-ray factors.

calculating and plotting Electron Charge Density (ECD), Electron technique.

The LMP2 correction to the HF DM is evaluated via a Lagrangian

distance. Allows the estimate of dispersive interactions up to infinite

Serves to reduce numerical noise in geometry optimizations.

Symmetry adapted Wannier Functions (SAWF) CRYSTAL09 prepares and transmits to CRYSCOR09 the SAWFs: these are local, orthonormal functions, equivalent to each other wrt crystal group operations, which span altogether the occupied Fock manifold.2 Their role in the LMP2 calculation is essential; they also permit a "chemical" analysis of the correlation energy.

Fast calculation of integrals Effective algorithms are used for calculating 2-electron integrals, based on a periodic extension of Density Fitting techniques and on the use of multipolar expansion methods.

Quasi-linear scaling of computational times Symmetry exploitation, efficient integration techniques, clever use of the locality Ansatz, allow LMP2 times to scale about linearly with N (compared to standard N^6 of canonical MP2).

LMP2 energy

The LMP2 energy per crystal cell is the main result of the calculation; its contribution to cohesive energies must be corrected for the Basis Set Superposition Error.3

Fix-index option

Serves to reduce numerical noise in geometry optimizations.

Lennard-Jones extrapolation

Allows the estimate of dispersive interactions up to infinite distance.

LMP2 Correction to Density Matrix (DM)
The LMP2 correction to the HF DM is evaluated via a Lagrangian technique.4 The corrected DM can be fed back to CRYSTAL09 for calculating and plotting Electron Charge Density (ECD), Electron Momentum Density (EMD), Compton Profiles, X-ray factors.

Essential bibliography


Symmetry-independent SAWFs of Boron Nitride Hexagonal BN

HF (CRYSTAL09) and LMP2 (CRYSCOR09) supercell calculations for a 3-L MgO slab (VTZ aug basis set)

Quasi-linear scaling of computational times

User’s Manual, Demo version, Tutorials

At the CRYSCOR web site (webmaster: M. Lorenz), you can get free of charge:

• The User’s manual (by A. Erba and M. Lorenz);
• A DEMO version of CRYSCOR09 (all functionalities, maximum 3 irreducible atoms);
• Examples of input and output;
• A collection of tutorials (from basic calculations to advanced applications).

CRYSCOR09

A computational tool for the ab-initio study of electron correlation in crystals

Web site: www.cryscor.unito.it
Contacts: cryscor@unito.it

CRYSCOR09 performs LMP2 calculations for non conducting systems periodic in 0,1,2 and 3 D. LMP2 means that standard Møller-Plesset theory at order 2 is adopted, in a local formulation similar to that used in the molecular MOLPRO package. Part of the integral package is taken from that code, on the basis of a joint agreement.

LMP2 is a well-assessed, parameter-free method: it provides a high-quality reference description of the energetics and electronic structure of covalent, ionic, molecular crystals. The Hartree-Fock (HF) zero-order solution plus all basic information concerning the system is provided by the periodic code CRYSTAL09 (see scheme below).

CRYSTAL09

Symmetry analysis
HF Eigenvalues & Eigenvectors
Fock matrix, Density matrix
Localization, Symmetrization
SAWFs
EDC, X-ray structure factors, EMD, Compton Profiles
Other Properties

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