CRYSTAL2010, a computational tool for the Solid State Chemistry

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The electronic structure and properties of crystals can be calculated ab initio with CRYSTAL at different levels of approximation ranging from Hartree-Fock (HF) to Kohn-Sham (KS) Density Functional Theory, including use of hybrid functionals. Expressing the wavefunction in terms of linear combinations of atomic orbitals (LCAO) allows easy interpretation of the electronic structure and direct comparison with molecular fragments.[1]

The release of the code presently distributed, CRYSTAL09,[2] enables fully automated and efficient search for minimum energy and transition state structures and the computation of a variety of properties including structural, elastic, piezoelectric, dielectric, magnetic and electronic properties, and the simulation of vibrational spectra. Extensive use of symmetry, in both the real and reciprocal space, and low computational requirements make the program efficient and suitable for the study of complex structures with ordinary computer facilities. Recent achievements in the parallelization of the code and use of parallel linear algebra libraries now permit large-scale calculations for systems containing thousands of atoms in the unit cell with good scalability over thousands of processors on High Performance Computers.

New developments also involve an efficient implementation of the Coupled-Pertubed (CP) HF/KS equations for the calculation of linear and nonlinear optical properties of insulators and semiconductors (electron polarization, dielectric and hyperpolarizability tensors). Application of the CPHF/CPKS method to the analytical calculation of various properties such as the piezoelectric tensor, infrared and Raman intensities is under development. In addition the program is now complemented with the possibility of doing post-Hartree-Fock calculations at the periodic Local MP-2 level, with the CRYSCOR code.[3] The program capabilities will be illustrated through examples of application.

References

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