

CRYSTAL: a modern tool for the *ab initio* study of crystalline solids. A focus on recent developments.

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The CRYSTAL program [1] has been developed since the 1970s and is one of the most widely used softwares for the quantum-mechanical study of crystalline solids. It computes the electronic structure of periodic systems within Hartree Fock, density functional or various hybrid approximations (global, range-separated and double-hybrids).

The Bloch functions of the periodic systems are expanded as linear combinations of atom centred Gaussian functions. As a consequence, global and range-separated hybrid functionals are accessible at a moderate computational cost.

CRYSTAL automatically handles space symmetry and allows calculation for system periodic in 3D (bulk), 2D(slabs), 1D(polymers) or, as a limiting case, 0D (molecule/cluster).

In the contribution some of the most recent developments of the code will be presented, including simulation of vibrational spectra (Infrared, Raman) with analytical intensities [2] and Linear and Non-Linear Optics (NLO) properties calculation (Second-Harmonic Generation, Pockels effect) for solids [3,4].

[1] R. Dovesi, R. Orlando, A. Erba, C. M. Zicovich-Wilson, B. Civalleri, S. Casassa, L. Maschio, M. Ferrabone, M. De La Pierre, P. D'Arco, Y. Noël, M. Causà, M. Rérat, B. Kirtman, *Int. J. Quantum Chemistry*, **114**(19), 1287-1317 (2014)

[2] L. Maschio, B. Kirtman, M. Rérat, R. Orlando, R. Dovesi, *J. Chem. Phys.* **139**, 164101 (2013)

[3] L. Maschio, M. Rérat, B. Kirtman, R. Dovesi, *J. Chem. Phys.* **143**, 244102 (2015)

[4] M. Rérat, L. Maschio, B. Kirtman, B. Civalleri, R. Dovesi, *J. Chem. Theory Comput.* (2015), *accepted* DOI: 10.1021/acs.jctc.5b00791