Ab initio Quantum-mechanical Calculation of Electron Charge-density in Crystals

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The *ab initio* quantum-mechanical CRYSTAL code [1] is one of the tools available for the calculation of the electronic structure and properties of crystals. It is based on a description of the wavefunction in terms of linear combinations of atomic orbitals (LCAO), which permits an easy interpretation of the electronic structure and a direct comparison with molecular fragments.

A large variety of properties of matter in the condensed phase can be calculated with the present release of the code, CRYSTAL03, even for systems of considerable size: a calculation of the electronic structure of the crambin protein ($P2_1$, 92 amino acid residues per cell) has been attained recently [2].

Molecular crystals are an important area of application of CRYSTAL. The use of a basis set of atomic orbitals is convenient for the calculation of the lattice energy and the characterization of hydrogen bonds, where the modifications in the electron charge density of the molecules due to the formation of the crystal can be investigated, along with their effect on the structure factors [3].

[1] Saunders,V.R., Dovesi R., Roetti C., Orlando R., Zicovich-Wilson C., Harison N.H., Doll K., Civalleri B., Bush I.J., D'Arco Ph., Llunell M., *CRYSTAL2003 user's manual*, University of Torino, Torino, 2003. [2] http://www.hpcx.ac.uk/about/newsletter/HPCxNews02.pdf, pages 10-12. [3] Spackman M. A., Mitchell A. S., *Phys. Chem. Chem. Phys.*, 2001, 3, 1518.

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