Geophysical Research Abstracts, Vol. 7, 09261, 2005
SRef-ID: 1607-7962/gra/EGU05-A-09261

CRYSTAL: a computational tool for solid-state science. Recent developments and applications

B. Civalleri

Dipartimento di Chimica IFM, Università di Torino, Italy

The CRYSTAL program [1] computes the electronic structure of periodic systems within Hartree Fock, density functional or various hybrid approximations. The Bloch functions of the periodic systems are expanded as linear combinations of atom centred Gaussian functions. Powerful screening techniques are used to exploit real space locality. The code may be used to perform consistent studies of the physical, electronic and magnetic structure of molecules, polymers, surfaces and crystalline solids. CRYSTAL is distributed to the scientific community since 1988 and the new release (CRYSTAL03) is now available [2]. Recent developments in CRYSTAL03 include: (a) the automated geometry optimization of the atoms in the unit cell at both HF and DFT level of theory; (b) calculation of dielectric properties (e.g. dielectric and piezoelectric constants).

Preliminary results on the calculation of vibrational frequencies and infrared intensities of crystalline compounds (e.g. quartz [3], calcite [4], pyrope [5]) will be reported. A few applications related to mineralogy and geochemistry will be discussed.

[1] CRYSTAL web site: http://www.crystal.unito.it

[2] V.R. Saunders, R. Dovesi, C. Roetti, R. Orlando, C. M. Zicovich-Wilson, N.M. Harrison, K. Doll, B. Civalleri, I.J. Bush, Ph. D'Arco, M. Llunell, CRYSTAL03 - User's Manual, University of Torino, (2003).

[3] F. Pascale, C.M. Zicovich-Wilson, F. Lopez-Gejo, B. Civalleri, R. Orlando, R. Dovesi, J. Comput. Chem. 25 (2004) 888; C.M. Zicovich-Wilson, F. Pascale, C. Roetti, V.R. Saunders, R. Orlando, R. Dovesi, J. Comput. Chem. 25 (2004) 1873

[4] M. Prencipe, F. Pascale, C.M. Zicovich-Wilson, V.R. Saunders, R. Orlando, R. Dovesi, Phys. Chem. Minerals 31 (2004) 559

[5] F. Pascale, C.M. Zicovich-Wilson, R. Orlando, C. Roetti, P. Ugliengo, R. Dovesi, J. Phys. Chem. B, submitted