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Preface: CECAM issue

Density functional theory (DFT) has grown enormously since its conceptual foundations were laid 30 years ago by Hohenberg and Kohn. DFT emphasizes the electron density of a system rather than the wave function, the traditional object of interest for quantum chemists. The powerful and practical scheme proposed by Kohn and Sham in 1965 formulated the many-body problem in a single-particle framework, through the use of an exchange and correlation (XC) potential. This potential is defined as a functional derivative of an XC energy functional of the electron density.

The first approximation to the XC potential and energy functionals was the so-called local density approximation which has been widely used for calculations of electronic properties of atoms, molecules and solids. Nonlocal, gradient-corrected, functionals for the XC terms in inhomogeneous systems have been developed more recently. The superiority of these functionals with respect to the homogeneous electron gas approximation has been demonstrated mainly in applications to molecular energetics.

Many accurate DFT studies have indeed been reported in recent years, for a broad range of compounds, including organic, inorganic, and organometallic molecules, clusters, crystalline solids, and for a broad range of properties: ground-state geometries, activation and dissociation energies, vibrational frequencies, dipole moments, polarisabilities, ionization and excitation energies, proton affinities, electrostatic potentials, chemisorption energies, etc.

The CECAM (Centre Européen de Calcul Atomique et Moléculaire) workshop on "Recent Developments in DFT, Computer Codes and Applications in Chemistry and Physics", held in Lyon, France (1–3 March 1994) was organized to promote discussions between specialists applying DFT methods to new fields of physics and chemistry and also researchers working on new code developments.

The invited participants have compared their experience with the various numerical techniques used in the different DFT codes. New developments have been reported, aiming at the calculation of physical properties such as NMR shifts or EPR parameters. Real chemistry involves solvents and activation barriers, which represent a challenge for quantum chemists. DFT methods are now able to handle the treatment of solvent effects and the determination of transition states along reaction profiles.

Participation in the Workshop was kept to a relatively small number to enhance personal contacts and to foster specialized discussions.

We are grateful to CECAM for the financial support of this Workshop and to all the participants for the very friendly atmosphere of those days, undoubtedly aided by the warm Lyon hospitality and the excellent Lyon gastronomy.

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CECAM Workshop

Recent Developments in DFT, Computer Codes and Applications in Chemistry and Physics

Lyon, France (1–3 March 1994)

Participants

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