



The Fundamentals of Electron Density, Density Matrix and Density Functional Theory in Atoms, Molecules and the Solid State (Progress in Theoretical Chemistry and Physics)

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This volume records the proceedings of a Forum on The Fundamentals of Electron Density, Density Matrix and Density Functional Theory in Atoms, Molecules and the Solid State held at the Coseners' House, Abingdon-on-Thames, Oxon. over the period 31st May - 2nd June, 2002. The forum consisted of 26 oral and poster presentations followed by a discussion structure around questions and comments submitted by the participants (and others who had expressed an interest) in advance of the meeting. Quantum mechanics provides a theoretical foundation for our understanding of the structure and properties of atoms, molecules and the solid state in terms their component particles, electrons and nuclei. (Relativistic quantum mechanics is required for molecular systems containing heavy atoms.) However, the solution of the equations of quantum mechanics yields a function, a wave function, which depends on the coordinates, both space and spin, of all of the particles in the system. This function contains much more information than is required to yield the energy or other property.

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