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DENSITY FUNCTIONAL THEORY OF MOLECULES, CLUSTERS, AND SOLIDS

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Rapid advances are taking place in the application of density functional theory (DFT) to describe complex electronic structures, to accurately treat large systems and to predict physical and chemical properties. Both theoretical content and computational methodology are developing at a pace which offers researchers new opportunities in areas such as quantum chemistry, cluster science, and solid state physics.

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Density Functional Theory (or DFT for short) is a potent methodology useful for calculating and understanding the molecular and electronic structure of atoms, molecules, clusters, and solids.

Density functional theory - Wikipedia

Density functional theory (DFT) is a computational quantum mechanical modelling method used in physics, chemistry and materials science to investigate the electronic structure (or nuclear structure) (principally the ground state) of many-body systems, in particular atoms, molecules, and the condensed phases.

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ELECTRONIC STRUCTURE AND PROPERTIES OF MOLECULES AND CLUSTERS: DENSITY FUNCTIONAL THEORY BASED APPROACH K.R.S. Chandrakumar Theoretical Chemistry Section, Chemistry Group, Bhabha Atomic Research Centre The author is the recipient of the Young Scientist Medal of the Indian National Science Academy (INSA), New Delhi for the year 2005. Abstract A theoretical basis for the concepts of chemical

Density Functional Theory for Beginners

The purpose of this site is to explain in a non-mathematical way what density functional theory is and what it is used for. I hope to familiarise the reader with the syntax of solid state theory and give a basic understanding of the related topics.