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Review: A Study and analysis on Density functional theory (DFT)

Shweta Kanungo[1], Ranjana Choudhary Ahirwar [2], Rajesh Babu Ahirwar [2], Deepi jain[3]**

1. Department of Biosciences, Acropolis Institute of Management Studies & Research, Indore (MP) India.
2.*Ips Academy, Institute of Engineering & Science Indore Madhya Pradesh 452012, India.
3. Department of Physics, ISR, IPS Academy Indore Madhya Pradesh 452012, India.
Email: ranjna.rajesh@gmail.com

Abstract

Density functional theory (DFT) has evolved into a central approach in computational quantum chemistry over recent decades. This theme issue, which marks the fiftieth anniversary of the Hohenberg–Kohn theorems, provides an overview of current developments and challenges in DFT research. Rather than being exhaustive, this theme issue aims to offer a broad view of many aspects of DFT. DFT is now widely accepted by both physicists and chemists as a valid theory and is often referred to as the standard method for periodic solids. In chemistry, DFT complements classical wave-function-based approaches, especially for systems with a large number of atoms.

Keywords: DFT, Electronic structure, NMR, UV, IR, TD-DFT, Energy, Frequency.