RECORDS & PROVISIONS

DFT: Density functional theory (DFT) is a quantum-mechanical (QM) method used in chemistry and physics to calculate the electronic structure of atoms, molecules and solids.

Open Access Review

Application of DFT Calculations in Designing Polymer-Based Drug Delivery Systems: An Overview

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Drug delivery systems transfer medications to target locations throughout the body. These systems are often made up of biodegradable and bioabsorbable polymers acting as delivery components. The introduction of density functional theory (DFT) has tremendously aided the application of computational material science in the design and development of drug delivery materials. The use of DFT and other computational approaches avoids time-consuming empirical processes. Therefore, this review explored how the DFT computation may be utilized to explain some of the features of polymer-based drug delivery systems. First, we went through the key aspects of DFT and provided some context. Then we looked at the essential characteristics of a polymer-based drug delivery system that DFT simulations could predict. We observed that the Gaussian software had been extensively employed by researchers, particularly with the B3LYP functional and 6-31G(d, p) basic sets for polymer-based drug delivery systems. However, to give researchers a choice of basis set for modelling complicated organic systems, such as polymer–drug complexes, we then offered possible resources and presented the future trend.

Keywords: **drug delivery system**; **DFT**; **polymer**; **nanocomposites**; **quantum mechanics**