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Review

Quantum Landscapes of Life: Leveraging DFT to Unravel Molecular Mechanisms in Bio-Chemical Catalysis

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ABSTRACT:

Density Functional Theory (DFT) has become a cornerstone computational approach for investigating the quantum mechanical basis of biochemical catalysis. By enabling a tractable description of electronic structure in complex molecular systems, DFT provides detailed insights into reaction pathways, activation energies, and molecular recognition processes in biological environments. This review outlines the theoretical foundations of DFT, including the Hohenberg–Kohn theorems and Kohn–Sham framework, followed by developments in exchange–correlation functionals and dispersion corrections. Applications to enzymatic catalysis particularly metalloenzymes are examined alongside discussions of hybrid QM/MM strategies and spin-state energetics. Finally, current limitations and emerging directions, such as machine learning integration and improved environmental modeling, are critically assessed.

Keywords:
DFT, Energetics, Environmental Modelling, Hornberg– Kohn Theorems, Kohn–Sham Framework

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