



Theoretical Biochemistry - Processes and Properties of Biological Systems (Theoretical and Computational Chemistry)

L.A. Eriksson

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Theoretical chemistry has been an area of tremendous expansion and development over the past decade; from an approach where we were able to treat only a few atoms quantum mechanically or make fairly crude molecular dynamics simulations, into a discipline with an accuracy and predictive power that has rendered it an essential complementary tool to experiment in basically all areas of science.

This volume gives a flavour of the types of problems in biochemistry that theoretical calculations can solve at present, and illustrates the tremendous predictive power these approaches possess.

A wide range of computational approaches, from classical MD and Monte Carlo methods, via semi-empirical and DFT approaches on isolated model systems, to Car-Parinello QM-MD and novel hybrid QM/MM studies are covered. The systems investigated also cover a broad range; from membrane-bound proteins to various types of enzymatic reactions as well as inhibitor studies, cofactor properties, solvent effects, transcription and radiation damage to DNA.

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