

Practical aspects of computational chemistry II : an overview of the last two decades and current trends

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Abstrak

This volume focuses on the association/dissociation of ion pairs in binary solvent mixtures, application of graph theory to determine the all possible structures and temperature-dependent distribution of water cluster, generalized-ensemble algorithms for the complex molecular simulation, QM/MD based investigation of formation of different nanostructures under nonequilibrium conditions, quantum mechanical study of chemical reactivity of carbon nanotube, covalent functionalization of single walled-carbon nanotube, designing of functional materials, importance of long-range dispersion interaction to study nanomaterials, recent advances in QSPR/QSAR analysis of nitrocompounds, prediction of physico-chemical properties of energetic materials, electronic structure and properties of 3d transition metal dimers, the s-bond activation reactions by transition metal complexes, theoretical modeling of environmental mercury depletion reaction, organolithium chemistry and computational modeling of low-energy electron induced DNA damage.