Overview of Theoretical Computational Tools: Selected multidisciplinary applications in Materials Science and Bio-Physical Chemistry

Carlton A. Taft
Centro Brasileiro de Pesquisas Físicas
Rua Dr. Xavier, Sigaud, 150, Urca, 22290-180
Rio de Janeiro, Brasil

Overview of Semi-Empirical, Hartree-Fock, Post-Hartree-Fock, Density Functional, Classical and Quantum (Monte Carlo and Molecular Dynamics), Plane waves, Monkhorst-Pack, Smearing, Pseupotentials (norm-conserving, Ultrasoft, PAW), Muffin-Tin approximations, FPLMTO, TD-DFT, GWA, SI, (Oniom, QM/MM), Docking, Virtual screening, PCA, ANN, KNN, HCA. Applications to Magnetism, conductivity, catalysis, adsorption, dissociation, coverage, defects, doping, supports, potential energy surfaces, electronic-band structure, structural parameters, charge distribution, density of states, energy gaps in sulphides, transition metals, oxides, fullerenes, nanotubes and other nano-structures. Interaction between biological receptors and ligands. Computer-aided design of advanced materials with technological potential.