Semiempirical models: on the way to combinatorial molecular design, large metal complexes architecture, and nanoscale bioassemblies

Alfredo Mayall Simas
UFPe - Brazil

Abstract

Semiempirical models are presently pushing the frontiers of quantum chemistry towards problems requiring, either thousands of calculations on systems of limited size, or a small number of calculations on systems contaning thousands of atoms. With emphasis on our recently developed models: RM1, or "Recife Model 1" and Sparkle, available in a number of widely distributed quantum chemistry softwares, we will exemplify several such applications which require the electronic wavefunction, e.g. the combinatorial theoretical design of molecules with large cross sections for two-photon absorption; lanthanide luminescence modeling; and protein enzymatic activity.