The Modern Role of NDDO-Based Semiempirical MO Theory

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NDDO-based MO theory has some characteristic strengths that define its role in modern research. These are primarily its applicability to large systems (100,000 atoms without local approximations[1] or 50,000 atom repeat-units in periodic calculations[2]), its good performance for one-electron properties[3] and excited states.[4] However, today's most widely used Hamiltonians suffer from a plethora of non-orthogonal two-center correction terms that improve the performance for weak interactions,[5] or even specific types of bond, such as C-C triple bonds.[6]

This lecture will describe software for very large-scale NDDO calculations and give examples of studies of charge transport in molecular electronic devices and biological systems.

The problem of the "misuse" of nucleus-nucleus potentials will be discussed and a "Feynman" dispersion correction introduced that does not depend on a modified internuclear potential.

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