

Poster presentation

Fast access to total energies

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A new computational method for the fast calculation of total energies is presented. Using classical Hückel molecular orbital (HMO [1]) theory and the partial equalization of orbital electronegativity (PEOE [2]) methodology it could be shown that heats of formation of large molecules might become accessible through quite simple means.

The new approach uses classical HMO calculation for the determination of bond orders, partial charges and bond energies in π -conjugated components. Furthermore, 2-dimensional Hückel problems are formulated and solved for isolated σ - and π -bonds. Assuming no charge interaction between σ - and π -orbitals, all non-conjugated parts of the considered molecule are iteratively allowed for charge transfer according to PEOE, which leads to the following scheme (Figure 1):

Correlating results from this procedure for a set of 201 organic molecules with total energies calculated by PM3 [3] lead to a very good agreement and a stability index of $R^2=0.991$. An incorporation into force fields for the inclusion of steric terms such as electrostatic interactions and van-der-Waals forces is planned.

References

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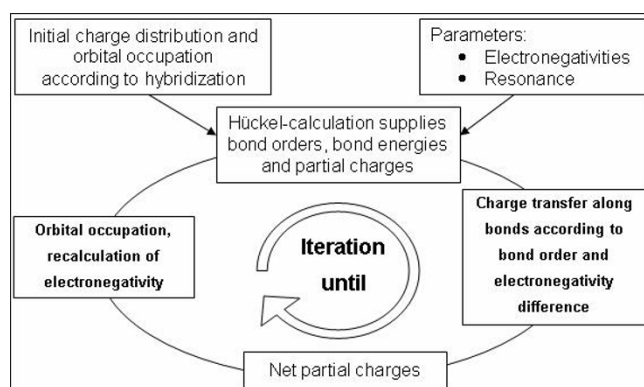


Figure 1