Pre-Born–Oppenheimer Molecular Structure Theory

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I shall present a theoretical and computational approach to the quantum mechanical description of molecules [1] which is free of approximations apart from assuming the validity of non-relativistic quantum theory. Conceptual questions about the reconstruction of the molecular structure in a fully quantum description will be discussed [2] and numerical results of exceedingly accurate bound and resonance states of the H_2 molecule will be presented [3]. Necessarily, I shall comment on the results and observations from the common standpoint of the Born–Oppenheimer separation of electrons and nuclei.

[1] E. Mátyus and M. Reiher, J. Chem. Phys. 137, 024104 (2012); B. Simmen, E. Mátyus, and M. Reiher, Mol. Phys. 111, 2086 (2013).

[2] E Mátyus, J. Hutter, U. Müller-Herold, and M. Reiher, Phys. Rev. A 83, 052512 (2011); J. Chem. Phys. 135, 204302 (2011); B. Simmen, E. Mátyus, and M. Reiher, J. Chem. Phys. 141, 154105 (2014).

[3] E. Mátyus, J. Phys. Chem. A 117, 7195 (2013).