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Electronic properties in liquid phase: combining many-body energy decomposition schemes with first principles molecular dynamics

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Abstract: The dynamics and electronic properties of systems in liquid phase are of fundamental interest for understanding chemical reactivity in solution. One important issue concerns the limitations of classical force fields for representing the interactions in liquid phase. Despite some progress, the accurate representation of polarization effects, dispersion interactions, and charge transfer processes in solution remains a challenge. First principles molecular dynamics, where the dynamics is generated with forces derived from electronic structure calculations is an interesting possibility to exploit. However, in this case, the results will be dependent on the adopted methodology for solving the electronic structure problem, which is usually based on density functional theory. The implementation, in liquid phase, of high accuracy *ab initio* methods, that can be currently applied to the calculation of gas-phase properties needs further theoretical developments. In this sense, the combination of many-body energy decomposition schemes (MBE) with first principles molecular dynamics should be considered as a promising alternative [1-3]. In this presentation, applications of first principles approaches for studying the structure, dynamics and electronic properties in liquid phase will be reviewed. Some emphasis will be given to the MBE/Molecular dynamics methodology for the calculation of the electronic spectra in liquid phase.

References:

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[3] Mata, RA; Cabral, BJC In *COMBINING QUANTUM MECHANICS AND MOLECULAR MECHANICS - SOME RECENT PROGRESSES IN QM/MM METHODS*, Edited by Sabin, JR; Brandas, E; Canuto, S. Adv. Quantum Chem., 59 (2010), 99-144. DOI: 10.1016/S0065-3276(10)59004-X