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R. Conte, G. Di Liberto, F. Gabas, M. Ceotto Semiclassical vibrational spectroscopy: the importance of quantum anharmonicity in supra-molecular systems.

Abstract

Semiclassical (SC) vibrational spectroscopy has been applied successfully to several molecular systems thanks to the possibility to regain quantum effects accurately starting from short-time classical trajectories.[1-5] Larger molecular and supra-molecular systems represent instead an open challenge in the field of semiclassical spectroscopy mainly due to the necessity to work in very high dimensionality. To start off the talk I will present some recent theoretical advances able to extend the range of applicability of SC vibrational spectroscopy to very high-dimensional systems.[6-7] Then, I will move to applications of semiclassical spectroscopy concerning the vibrational features of water clusters and two supra-molecular systems involving glycine.[8-9] These applications will point out the importance of a multi-reference, dynamical approach able to reproduce quantum anharmonicities without employing any ad-hoc scaling factor.

- [1] M. F. Herman, E. Kluk, *Chem. Phys.* 1984, 91, 27.
- [2] A. L. Kaledin, W. H. Miller, *J. Chem. Phys.* 2003, 118, 7174.
- [3] M. Ceotto, S. Atahan, G. F. Tantardini, A. Aspuru-Guzik, *J. Chem. Phys.* 2009, 130, 234113.
- [4] R. Conte, A. Aspuru-Guzik, M. Ceotto, *J. Phys. Chem. Lett.* 2013, 4, 3407.
- [5] F. Gabas, R. Conte, M. Ceotto, *J. Chem. Theory Comput.* 2017, 13, 2378.
- [6] M. Ceotto, G. Di Liberto, R. Conte, *Phys. Rev. Lett.* 2017, 119, 010401.
- [7] G. Di Liberto, R. Conte, M. Ceotto, *J. Chem. Phys.* 2018, 148, 014307.
- [8] G. Di Liberto, R. Conte, M. Ceotto, *J. Chem. Phys.* 2018, 148, 104302.
- [9] F. Gabas, G. Di Liberto, R. Conte, M. Ceotto, to be submitted.