

Title: **Semiclassical Molecular Dynamics for Spectroscopic Calculations of Complex Systems**

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Abstract:

I will present some novel semiclassical methods for spectroscopic calculations. These approaches can be employed for spectroscopic calculations of gas-phase molecular and supramolecular systems up to hundreds of degrees of freedom, as well as to condensed phase systems. Some methods are based on a “divide-and-conquer” approach, where the full dimensional spectra are obtained as a composition of several lower dimensional ones. Others exploit hierarchically the different levels of accuracy of different semiclassical propagators. For instance, in a system-bath problem lower semiclassical accuracy is dedicated to the bath, while the system is treated with higher accuracy and the system spectrum is eventually singled out.

All methods are amenable for ab initio molecular dynamics simulations.

References

1. F. Gabas, G. Di Liberto, R. Conte, and M. Ceotto, *Chemical Science* **9** (41), 7885-8026 (2018);
2. X. Ma, G. Di Liberto, R. Conte, W. L. Hase, and M. Ceotto, *JCP* **149**, 164113 (2018)
3. M. Micciarelli, R. Conte, J. Suarez, and M. Ceotto, *JCP* **149**, 064115 (2018);
4. M. Buchholz, F. Grossmann, and M. Ceotto, *JCP* **148**, 114107 (2018);
5. G. Di Liberto, R. Conte, and M. Ceotto, *JCP* **148**, 104302 (2018);
6. G. Di Liberto, R. Conte, and M. Ceotto, *JCP* **148**, 014307 (2018);
7. M. Buchholz, F. Grossmann, and M. Ceotto, *JCP* **147**, 164110 (2017);
8. M. Ceotto, G. Di Liberto, and R. Conte, *PRL* **119**, 010401 (2017);
9. F. Gabas, R. Conte, and M. Ceotto, *JCTC* **13**, 2378-2388 (2017);
10. G. Di Liberto, M. Ceotto, *JCP* **145**, 144107 (2016);
11. M. Buchholz, F. Grossmann, M. Ceotto, *JCP* **144**, 094102 (2016);