SEMISOFT: A web-platform interface for vibrational spectroscopy calculations

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In this presentation I will introduce a free software web-platform interface[1] for the simulation of the vibrational power spectra, i.e. the classical vibrational density of states, which is the collection of all possible molecular fundamental spectroscopic transitions. The web-platform relies only on a single molecular dynamics classical trajectory, which can be obtained with any type of molecular dynamics software, including Born-Oppenheimer ab initio molecular dynamics trajectories. The audience will be introduced to the usage of the web-platform. I will show how the trajectory information can be uploaded and employed for generating the vibrational spectra. Several examples will be shown for different chemical systems, ranging from gas phase isolated molecules to condensed phase ones, such as solvated or adsorbed molecules.[2]

References

[1] http://semisoft.unimi.it/

[2] R. Conte, M. Gandolfi, D. Moscato, C. Aieta, S. Valtolina, M. Ceotto, *J. Comput. Chem.* **2025**, *46, e70118.*