

## Title: Quantum Mechanical **Methods for Spectroscopic Calculations of High Dimensional Molecular 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.

All methods are amenable to ab initio molecular dynamics simulations.

### **References**

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