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Understanding Dynamic Calculations of Anharmonic Infrared Spectra

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The infrared spectrum of a molecular system is traditionally calculated from energy derivatives at its equilibrium geometry. Such methods are inherently limited to a single static point, and cannot describe anharmonic potential features such as the ergodic double-well. A more recent approach is to simulate classical vibration with Born-Oppenheimer molecular dynamics, freely exploring the potential surface. The trajectory is then processed into an infrared spectrum using the Fermi Golden Rule. I will explain why this approach works, and compare its results on toy and real systems to that of static methods. I will also discuss the role of the most important numerical parameters.

Author: ANDERSSON, Åke

Presenter: ANDERSSON, Åke

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