Semiclassical molecular dynamics for IR spectroscopy of molecules and materials

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I introduce a recently developed theory for performing IR spectroscopy with semiclassical molecular dynamics.[1,2] I start by showing the theoretical details of the theory, demonstrating its high accuracy and computational effectiveness. Then, I present some applications to gas-phase molecules, showing that the method can straightforwardly be applied to large dimensional solvated systems and materials.
In the final part of the talk I compare the capabilities of this semiclassical method to those of very popular path-integral methods like centroid molecular dynamics and ring polymer molecular dynamics, demonstrating why semiclassical approaches are a better choice for vibrational spectroscopy calculations and should be the preferred ones.

[1] C. Lanzi, C. Aieta, M. Ceotto, R. Conte J. Chem. Phys. **160**, 214107 (2024).
[2] C. Lanzi, C. Aieta, M. Ceotto, R. Conte J. Chem. Phys. **163**, 024122 (2025).