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Accurate determination of infrared spectroscopy in hydrogen-rich materials

The aim of this work is the calculation of vibrational properties of hydrogen-rich materials where Nuclear Quantum Effects play an important role. The computational methods are based on Molecular Dynamics simulations combined with Quantum Monte Carlo (QMC) for the electronic part and a Langevin thermostat correlated according to the covariance matrix of QMC nuclear forces. In particular, we want to assess the influence of the Langevin thermostats over dynamical properties such as vibrational spectra.

Field

Condensed Matter Physics

Language

English

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