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Periodic Density Functional Theory for the Prediction of Terahertz Spectra

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Accurate simulation of low-frequency fundamental and lattice modes, as obtained from terahertz and far-infrared spectroscopy of crystalline molecular solids, has long proved difficult. Long-range intermolecular interactions in the solid-state are notoriously difficult to model, resulting in deviation from experimental frequencies obtained from thin films and aerosols. In this talk, we present a series of calculations using the periodic DFT code CRYSTAL17 now installed on the parallel ASCI environment. These studies have yielded highly accurate simulated far-IR spectra (frequencies and intensities) for comparison to molecular crystal spectra measured at the THz and Far-IR beamline. The results have allowed the assignment of lattice vibrations pertaining to astrophysical ice and forensic samples, many for the first time. Potential for the coupled theory-to-experiment method applied to molecular organic framework (MOF) and pharmaceutical systems will be discussed.

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