AB-INITIO INVESTIGATION OF TERAHERTZ VIBRATIONAL MODES IN MOLECULAR CRYSTALS

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We use the CASTEP ab-initio density-functional perturbation theory code[a] to investigate the properties of terahertz-frequency vibrational modes in crystalline systems. We will discuss the strong mixing of molecular and phonon modes in hydrogen-bonded crystals[b], and also discuss ongoing work where we study nonlinear interaction between intense THz light and molecular crystals.

[a] S. J. Clark, et al., Z. Kristallographie **220,** 567 (2005)
[b] P. Uhd Jepsen and S. J. Clark, Chem. Phys. Lett. **442,** 275 (2007)