

Abstract Submitted
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First Principles Simulations of THz Spectra of Acephate: Insight Into the Phonon Signatures. YIMING ZHANG, XIHONG PENG, YUNQING CHEN, SAROJ NAYAK, X.-C. ZHANG, Rensselaer Polytechnic Institute, RENSSELAER POLYTECHNIC INSTITUTE TEAM — Acephate is an insecticide that kills insects by disrupting nervous system functions. THz spectroscopy offers a unique tool for detecting trace amount of these materials. Using a combination of solid state first principles simulations and gas phase quantum mechanical modeling we have studied phonon spectra of acephate compound. This talk will present a detailed vibrational spectra analysis over a wide range of frequency and our computational data will be compared with available experimental results.

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