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Abstract:Terahertz absorption spectrum (0.5-4.0 THz) of L-alanine in the solid phase was measured by terahertz time-domain spectroscopy at room temperature. Simulations utilizing gaseous-state and solid-state theory were performed to determine the origins of the observed vibrational features. Our calculations showed that the measured features in solid-state materials could be well understood by considering the crystal packing interactions in a solid-state density functional theory calculation. Furthermore, intermolecular vibrations of L-alanine are found to be the dominating contributions to these measured spectral features in the range of 0.5-4.0 THz, except that located at 3.11 THz.
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