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Title:Calculation of infrared/raman spectra and dielectric properties of various crystalline poly(lactic acid)s by density functional perturbation theory (DFPT) method
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Abstract:We calculated infrared (IR) and Raman spectra of poly(lactic acid) (PLA) polymorphs by employing density functional perturbation theory (DFPT) and a plane wavebasis set. Significant different characteristics are found in the calculated spectra of poly(l-lactic acid) (PLLA) α-form and PLLA/poly(d-lactic acid) (PDLA) stereocomplex (sc) form. Particularly in the carbonyl stretching region, there is only one sharp peak in the sc-form while there are five peaks in the PLLA α-form. A low wavenumber (65 cm ⁻¹) vibration band of α-PLLA observed in a previous terahertz time-domain spectroscopy study was reproduced in the calculated solid-state PLLA spectra. This band could not be obtained by using DFT (B3LYP/6-31G*) simulation on a single PLA oligomer chain and had been attributed to lattice vibrations in the crystal. The permittivity and polarizability tensors of PLA single crystals were also obtained using the DFPT method and were found to be anisotropic. © 2012 American Chemical Society.
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Uncontrolled terms:A-plane - D-Lactic acid - Density functional perturbation theory - DFPT - Infrared and Raman spectra - Oligomer chains - PLLA - Polarizability tensor - Poly L lactic acid - Poly(lactic acid) - Polylactic acids - Stereocomplexes - Stretching region - Terahertz time domain spectroscopy - Vibration bands - Wave numbers

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