Abstract Submitted
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Convergence of the phonon energy in two-dimensional atomic crystal of lead[1] JIA-AN YAN, Department of Physics, Astronomy and Geosciences — Accurate phonon energies are important for the study of two-dimensional (2D) atomic crystals. Using the 2D honeycomb lattice of lead (Pb) as a model system, we studied the convergence of the phonon energies on several important parameters in supercell calculations based on the density-functional perturbation theory as implemented in Quantum Espresso code. These parameters include the plane wave cut-off energy, the vacuum space size, the charge density cut-off, and FFT grid. The tested pseudopotentials (PPs) include the widely used Troullier-Martin (TM), Hartwigsen-Goedeker-Hutter (HGH), Projector Augmented-Wave (PAW), and ultrasoft pseudopotential (USPP), with the same PBE exchange-correlation functional. Surprisingly, the phonon energies calculated using these PPs exhibit quite distinct dependence on those parameters. Specifically, for both TM and USPP PPs, the phonon energies at the Brillouin zone center exhibit oscillations and even large negative phonon modes with the increase of the vacuum size. In contrast, the HGH and PAW PPs show fast and stable convergence with the same settings. The origin of these oscillation will be discussed.

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