Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials for

Electron-phonon interaction and superconductivity in the high-pressure cI16 phase of lithium from first-principles

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1. Formation energy per atom of cI16 phase

We calculated the formation energy per atom of c116 phase with different pressures with DFT method. The reference energy is from the ground state bcc phase Li under zero pressure. We present the formation energy information in the Figure. S1.

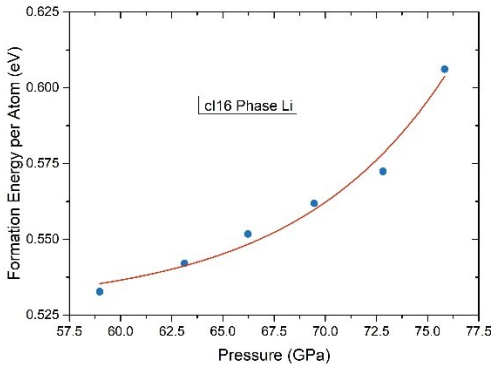

Figure. S1. The formation energy per atom of cI16 phase Li versus the pressure. The referenced energy is from the ground state bcc phase Li.

2. Different exchange-correlation functional effect in the electronic band structures and phonon dispersions

Here, the pseudopotentials based on the projector augmented wave (PAW)[1] method were adopted. We adopt different exchange-correlation functionals - local density approximation (LDA)[2] and Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA)[3] - in Vienna ab-initio simulation package (VASP)[4,5]. At the same time, we also did the DFT calculation in VASP with Heyd–Scuseria–Ernzerhof (HSE)[6,7] approach. The cutoff of kinetic energy for wave functions was set at 500 eV and the energy convergence threshold was set as 10^{-8} eV. The Monkhorst[8]-Pack k-meshes of $8 \times 8 \times 8$ were used to sample the Brillouin Zone (BZ). We applied the density functional perturbation theory (DFPT)[9] method in VASP to calculate the phonon dispersions via the PHONOPY[10] package. The Hellmann–Feynman force tolerance is $10^{-6}\ eV\ Å^{-1}$. We showed the calculation results of the electronic band structures and phonon dispersions of cI16 phase Li under different pressures in Figure. S2. and Figure. S3., respectively.

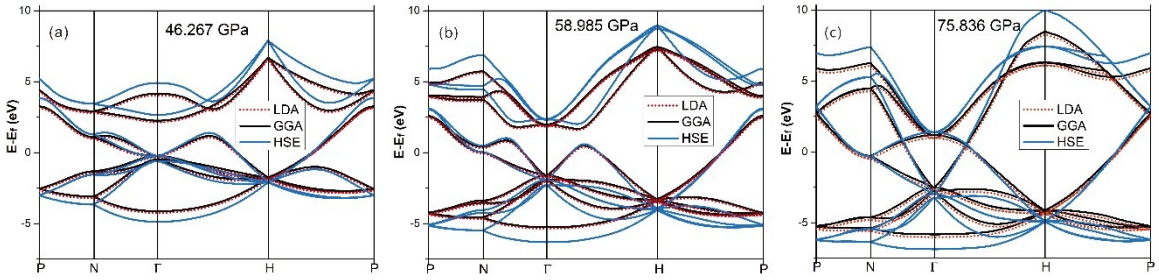

Figure. S2. The electronic bands structures of cI16 Li under different pressure. The XC functionals LDA, GGA and HSE06 are employed in VASP.

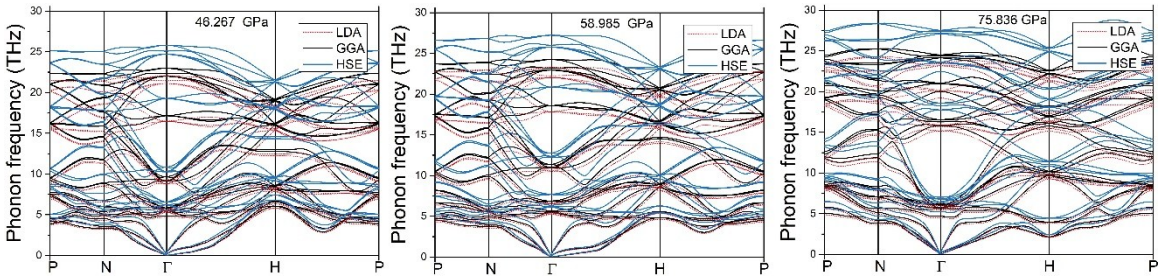

Figure. S3. The phonon dispersions of cI16 Li under different pressure. The XC functionals LDA, GGA and HSE06 are employed in VASP.

From the results we can see that the electronic band structures near the Fermi level, where the electron-phonon interaction has the most impact on the superconducting properties, are nearly identical for all three functionals, with appreciable difference only in energy bands far from the Fermi level. In the phonon dispersions, the major contributors to the electron-phonon interaction - the low-frequency acoustic phonons, are also less influenced by the choice of the functionals. Based on these observations, we expect small impact of different functionals on the calculated results.

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