Supplementary Materials for

Superconductivity of monolayer functionalized biphenylene with Dirac cone

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I. Final relaxation positions of the bridge and top configurations with Li

We study the relaxation properties of Li-deposited biphenylene. There are three sites with high symmetry: hollow, top, and bridge coverages of the biphenylene, with the Li atom lying above the center of the carbon rings, above the C atom, and above the center of the C-C bond, respectively. In the first instance we placed Li atoms over top or bridge sites on the membranes. After full relaxation, it is clearly seen that Li atoms move to the hollow sites, with the results shown in Figs. S1,S2. It means that Li atoms on the top and bridge sites of biphenylene are not stable, and the hollow sites above the center of the carbon rings are preferred.

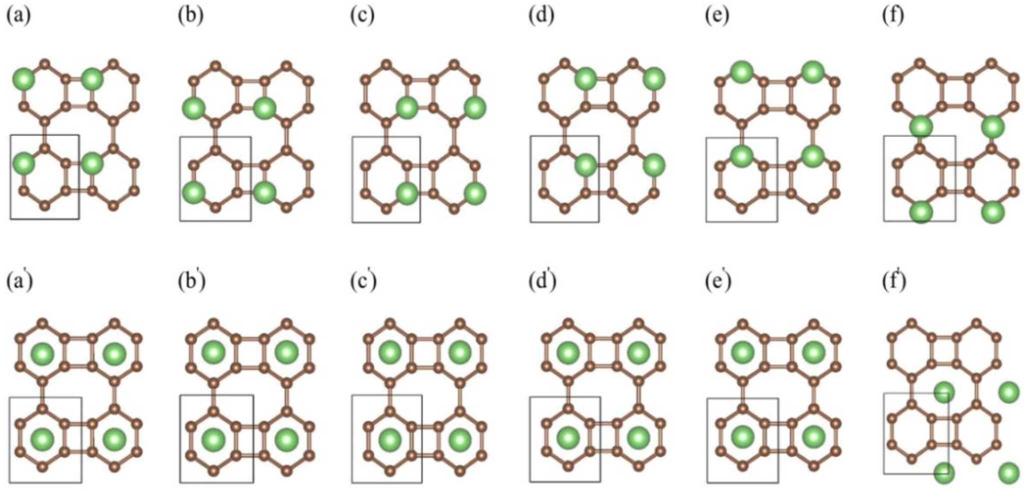

Fig. S1: (a-f) Initial positions of Li atoms on top sites. (a'-f') Corresponding final positions of Li atoms after full relaxation. It can be seen that Li atoms lying on the top sites move to the hollow sites. Brown balls represent carbon and green balls are Li atoms.

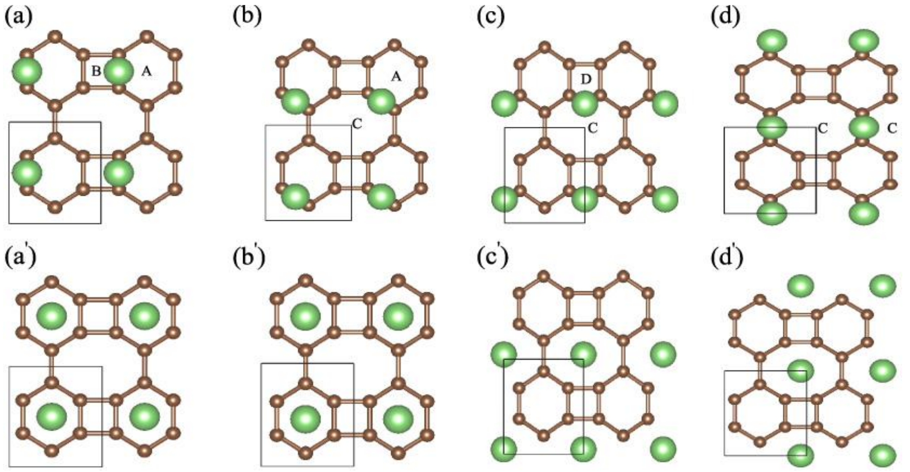

Fig. S2: (a-d) Initial positions of Li atoms on bridge sites. (a'- d') Corresponding final positions of Li atoms after full relaxation. It can be seen that Li atoms lying on the bridge sites move to the hollow sites.

II. Phonon spectra with Li deposited on the hollow sites of six- and eight-carbon rings.

The adsorption energies are 1.725, 1.900 and 1.897 eV for one Li adsorbed on four-, six- and eight-membered carbon rings, respectively. The results indicate that Li possesses almost the same stability on the hollow positions of the six- and eight-membered carbon rings, but are more stable than that on the hollow site of four-membered carbon rings. Our results support the idea that Li will prefer to occupy a position with a larger space.

In order to further investigate the dynamical stability, we calculate the phonon spectra for Li lying on the hollow positions of six- and eight-membered carbon rings respectively, with the results shown in Fig. S3. We find that there is no imaginary frequency for Li lying on the hollow positions of six-membered carbon rings. However, for Li lying on the hollow positions of eight-membered carbon rings, the imaginary frequency of about $-41\,\mathrm{cm}^{-1}$ appears, indicating that the lattice is dynamically unstable, see Fig. S3. Thus, in the following, we study the properties for the structure of biphenylene with Li-deposited on the hollow positions of six-membered carbon rings.

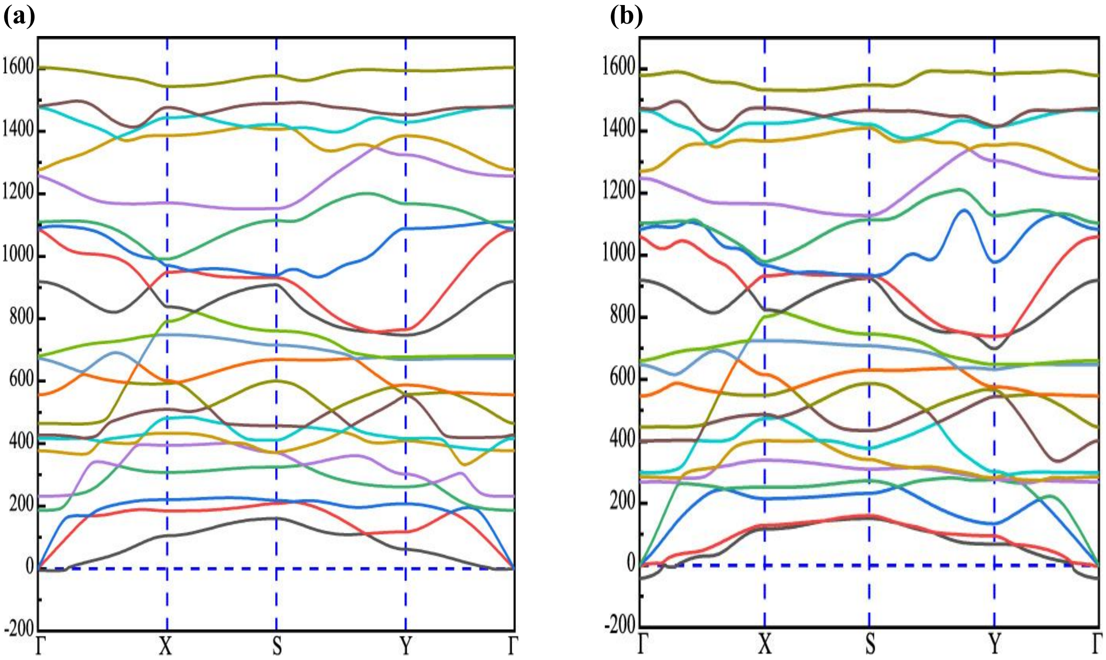

Fig. S3: Phonon spectra with Li deposited on the hollow sites of (a) six- and (b) eight-carbon rings.

III. Phonon spectra under different biaxial tensile strains

We calculate the phonon spectra of Li-deposited biphenylene under different biaxial tensile strains and find that there is no imaginary frequency in the phonon spectra at biaxial tensile strains up to 12%. When the biaxial tensile strain is lager than 12%, the imaginary frequency appears, indicating that the lattice is no longer stable. The phonon spectra at ε =12% and ε =13% biaxial tensile strains are listed in Fig. S4. It can be concluded that biaxial tensile strains of ε = 12% is the highest tensile strain that can be applied to Li-deposited biphenylene. Thus, we only investigate the properties of Li-deposited biphenylene under biaxial tensile strains below 12% in this work.

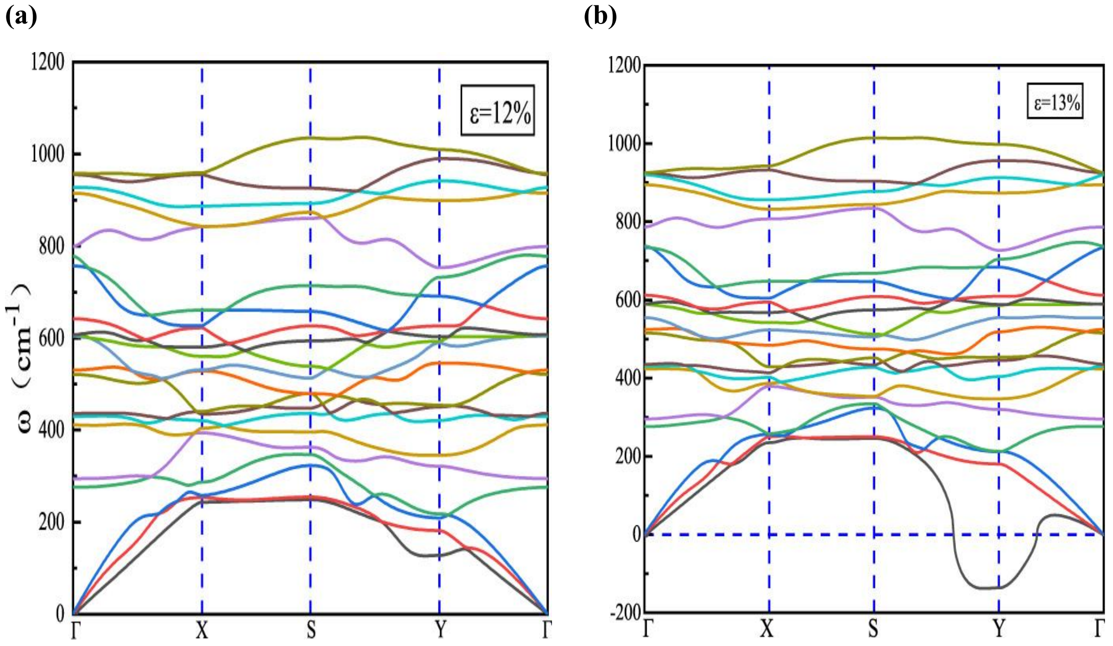

Fig. S4: Phonon spectra at (a) 12% and (b) 13% biaxial tensile strains.