Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information For

OPGs: Promising Anode Materials with High Specific Capacity and Rate Capability for Li/Na Ion Batteries

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Supplementary Figures:

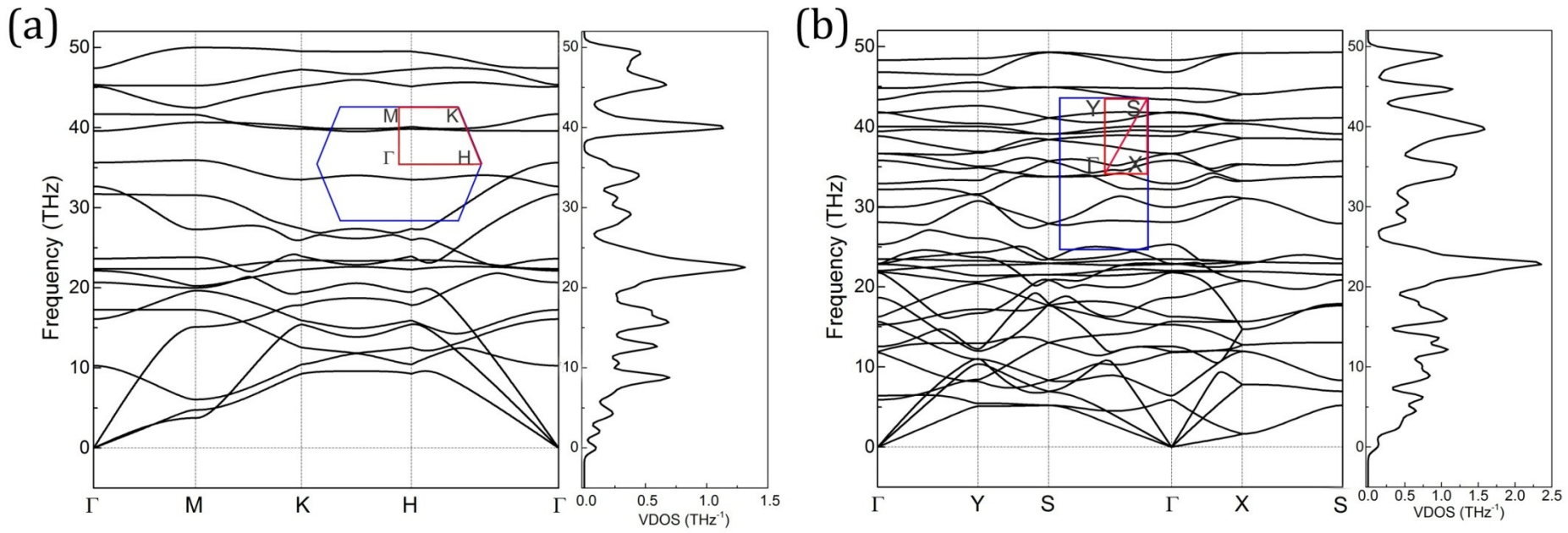

Figure S1. Phonon dispersion and vibration DOS of (a) OPG_L and (b) OPG_Z. Inset: The first Brillouin zones and high symmetry points of OPG-L and OPG-Z.

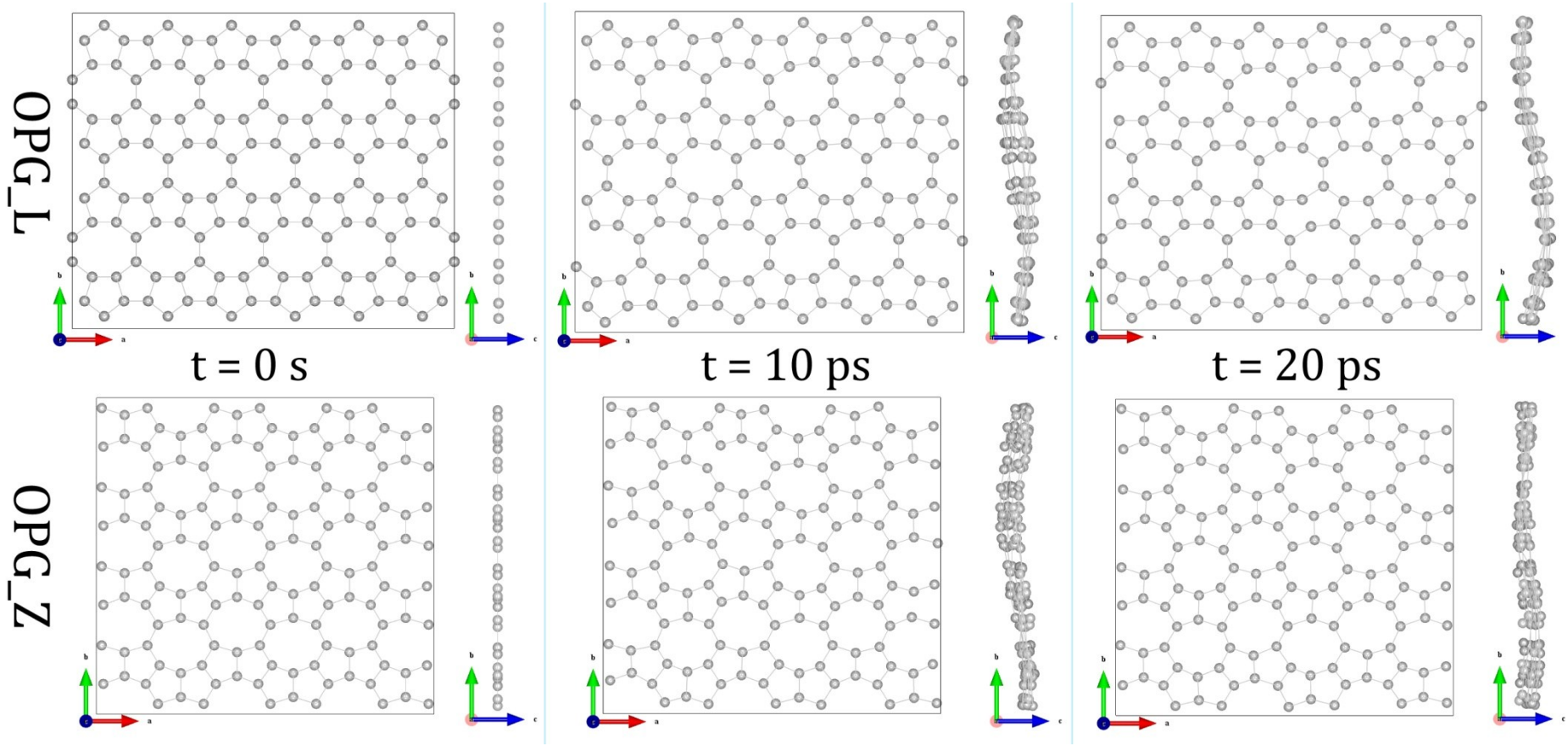

Figure S2. Top (left) and side (right) views of snapshots for OPGs at temperature of 1000 K. In each partial，left show the top view and right side view.

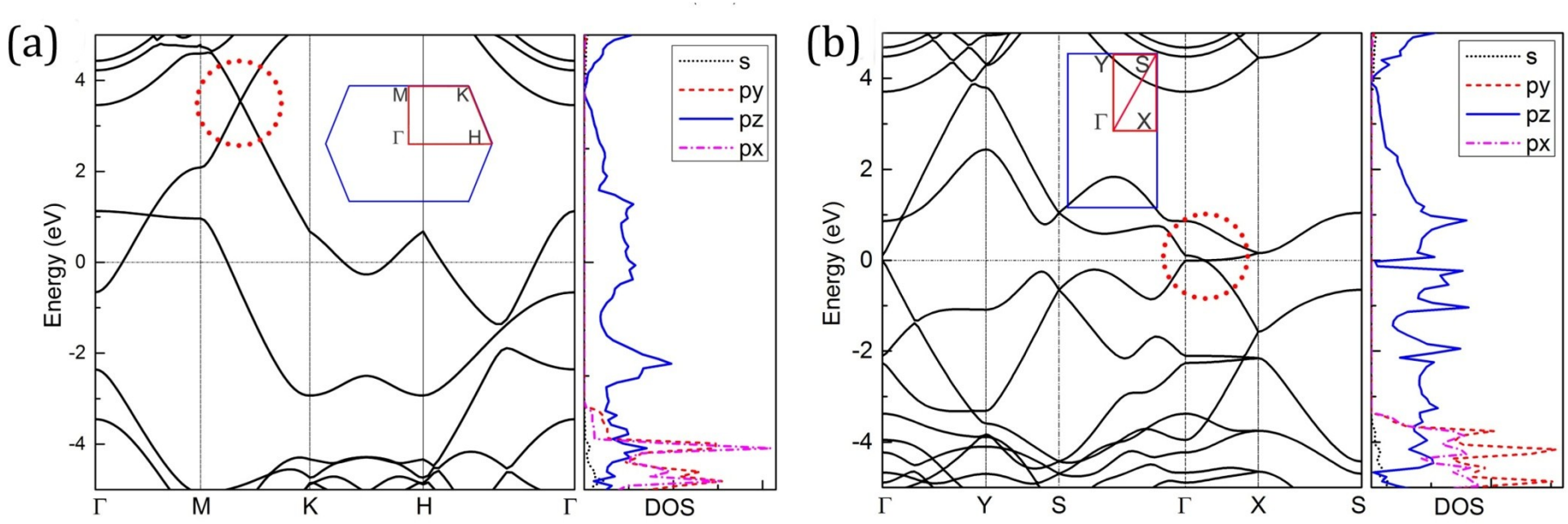

Figure S3. Electronic band structures and DOS of (a) OPG_L and (b) OPG_Z. The dirac-like points are marked in red dotted circles.

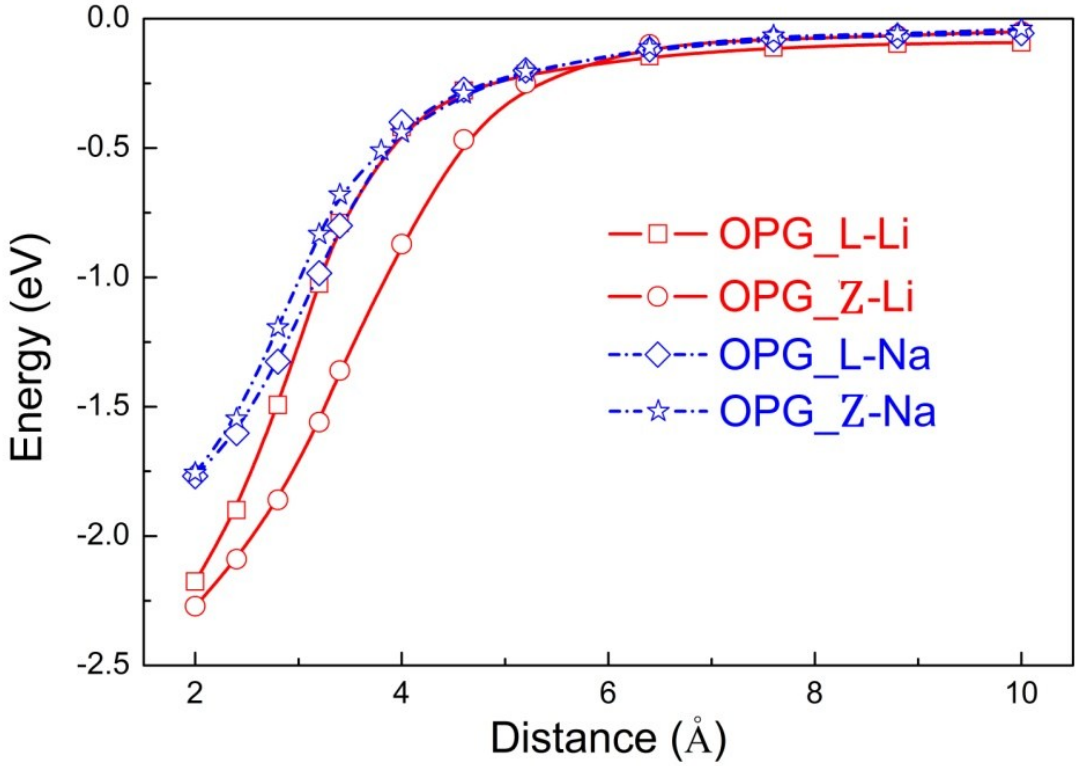

Figure S4. Relative energy of Li/Na adsorbed on the OPGs against the distance between Li/Na and OPG surfaces.

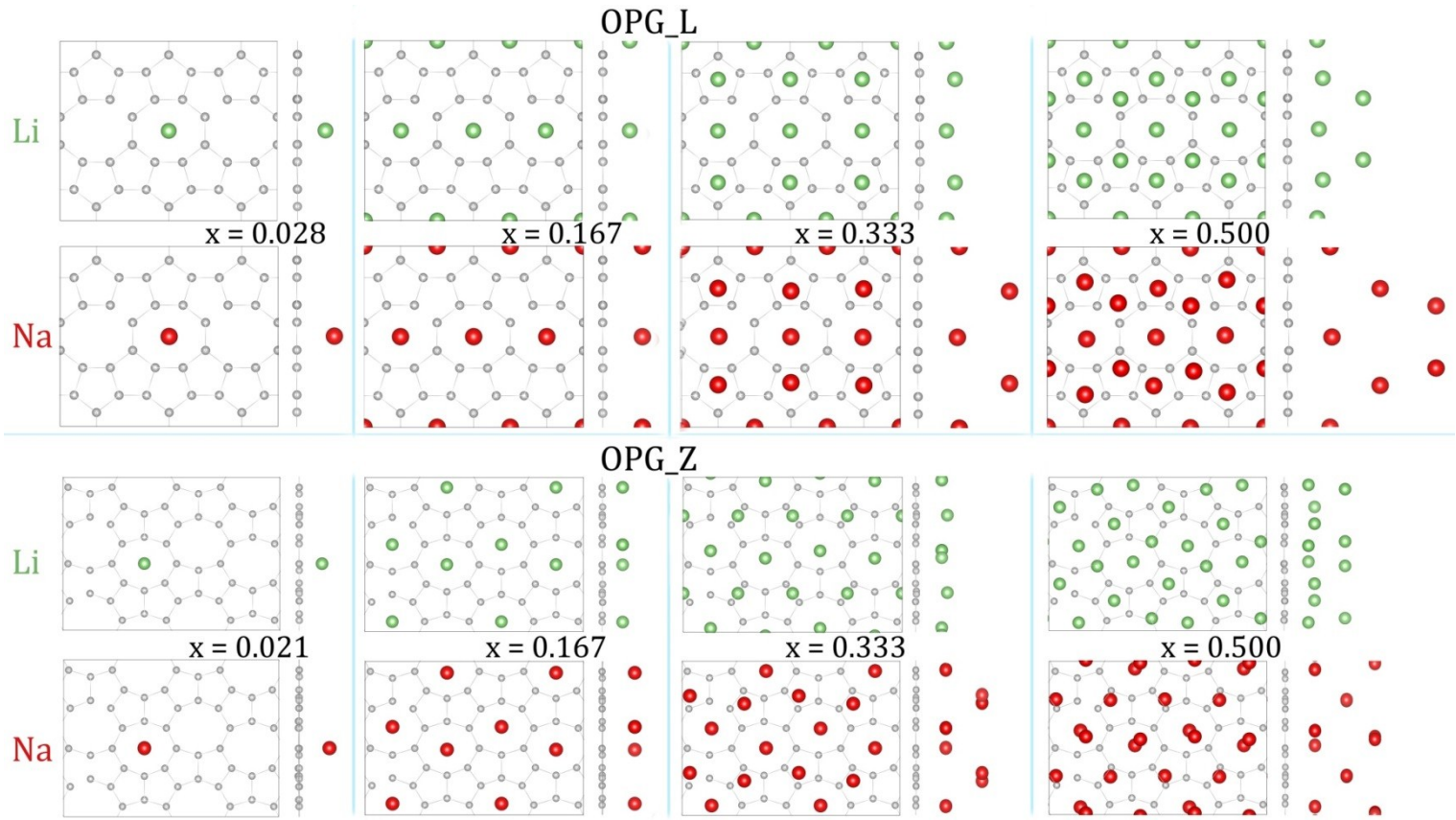

Figure S5. Structures of OPGs with various Li/Na concentrations. In each partial， left show the top view and right side view.

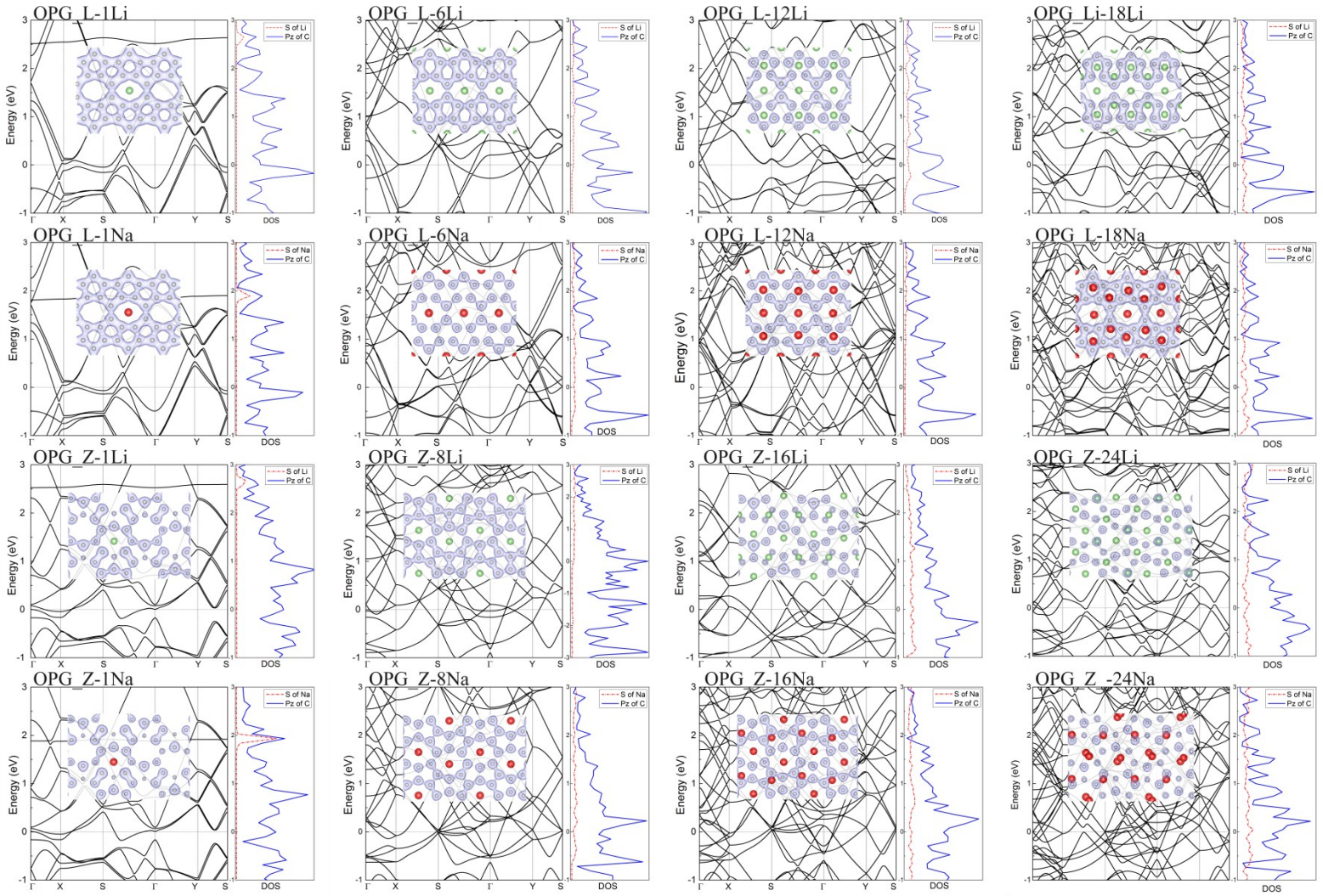

Figure S6. The electronic band structures and DOS of OPGs with different Li/Na contents. Insets show corresponding spatial electronic distribution around the Fermi-level. The isosurface (grey) value is 0.01 e/Å^3.

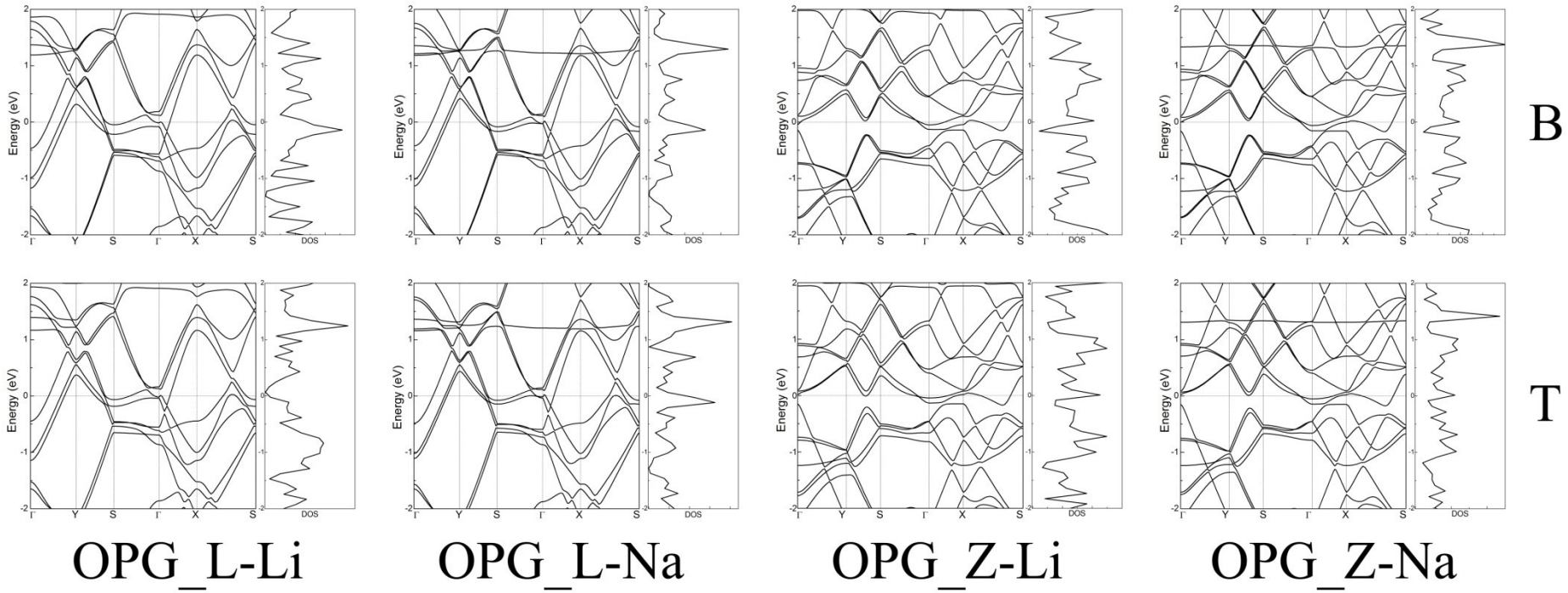

Figure S7. Electronic band structures and DOS of OPGs absorbed with a Li/Na atom on B- or T-sites. For both the B- and T-sites, there are several different adsorption structures. Here, we just show one of them because the results are almost indistinguishable.