Electronic Supplementary Information (ESI)

Comparative First-Principles Study of the Lithiation, Sodiation, and Magnesiation of Black Phosphorus for Li-, Na-, and Mg-Ion Batteries

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Figure S1. Radial distribution function (RDF) of MxP. (M = Li, Na and Mg).
**Figure S2.** Formation of tunnel-like channels in black phosphorus during lithiation, sodiation and magnesiation. Here, for clarity, volume expansion of black phosphorus induced by the lithiation, sodiation, and magnesiation is ignored. The red, pink, navy blue and green balls represent P, Li, Na and Mg atoms, respectively.
Figure S3. Equation of states and bulk moduli of black phosphorus and M$_2$P (M = Li, Na and Mg). Here, the bulk modulus was calculated by fitting Murnaghan equation of states for the energy curve as a function of volume.
**Figure S4.** Calculated formation energy of MxP systems (M = Li, Na, and Mg). Here, the inset in each figure correspond to data for layered black phosphorus region at low M concentrations and the data include all of the possible configuration of interaction.