

Sodium-Induced Reordering of Atomic Stacks in Black Phosphorous

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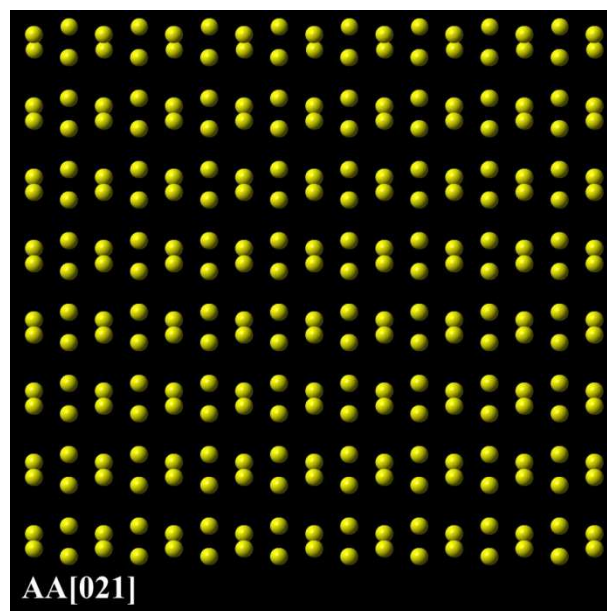


Figure S1 Atomic model for AA stacking BP with the $[021]$ projection.

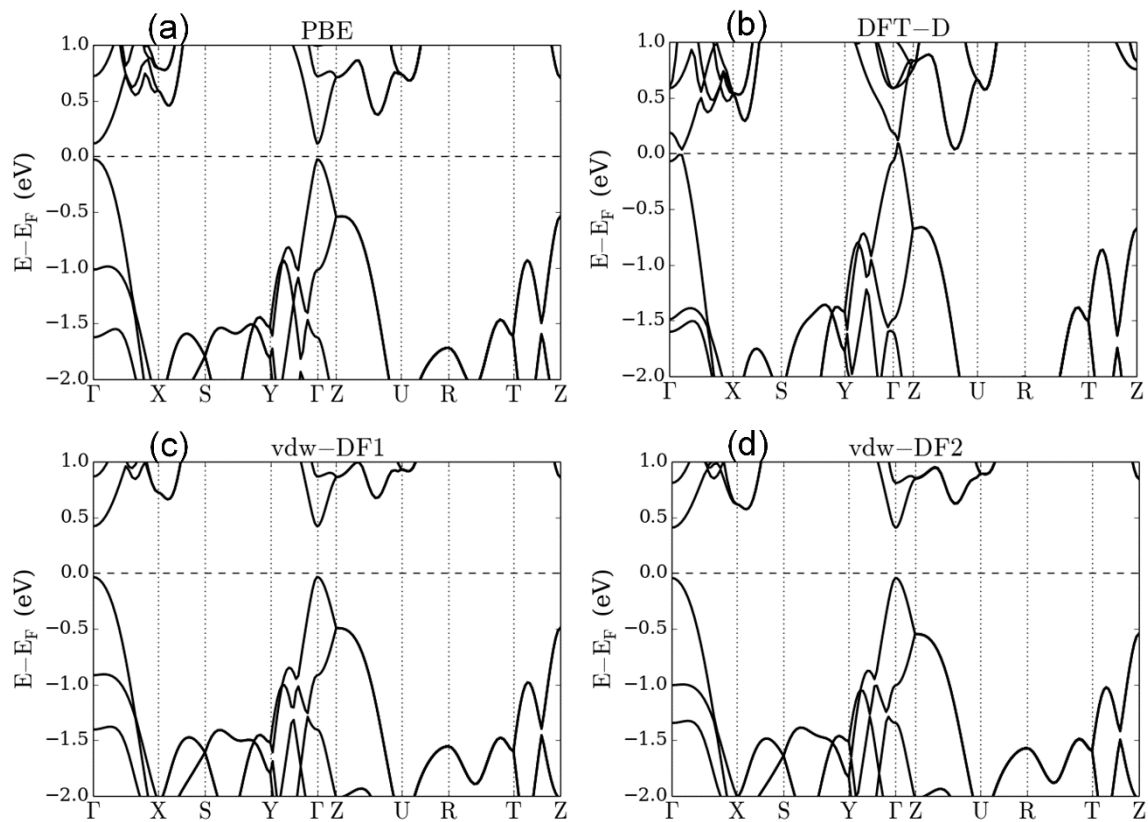


Figure S2 Band structure for bulk BP calculated by using (a) PBE functional, (b) DFT-D empirical van der Waals correction, and first principles van der Waals correction (c) vdw-DF1, and (d) vdw-DF2.

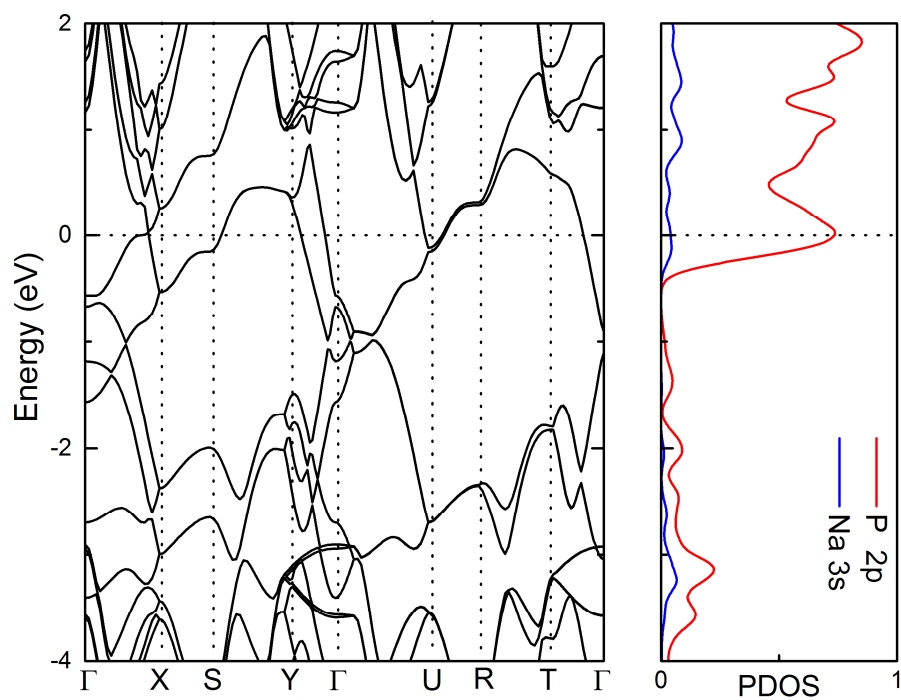


Figure S3 Band structure and partial density of states (PDOS) for the bulk BP with AC stacking order after sodium intercalation.

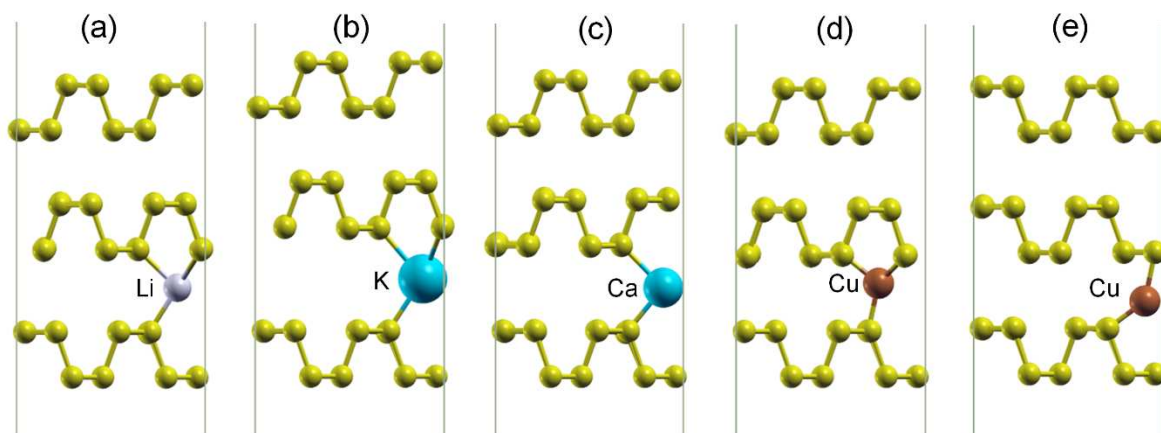


Figure S4 Atomic structure for trilayer BP intercalated by (a) Li, (b) K, (c) Ca and (d) Cu by using vdw-DF1 van der Waals correction.

Movie S1 Energy, volume and structure evolution for bulk BP with one layer sodium intercalation in the structure relaxation process.

Movie S2 Energy, volume and structure evolution for bulk BP with two layer sodium intercalation in the structure relaxation process.