Supporting information

Structural, elastic, and electronic properties of chemically functionalized boron phosphide monolayer

Tuan V. Vu, A.I. Kartamyshev, Nguyen V. Hieu*, Tran D.H. Dang, Sy-Ngoc Nguyen, N.A. Poklonski, Chuong V. Nguyen, Huynh V. Phuc, Nguyen N. Hieu*

*Corresponding authors: nvhieu@ued.udn.vn; hieunn@duytan.edu.vn.

Table S1. Coordinates of atoms in the functionalized BP monolayer with Br and Cl atoms. $Cl(Br)_{B/P}$ indicates the Cl(Br) bonded directly to B/P atom.

Configuration	Atom	x	y	z
Cl–BP–Cl	B	0.33333	0.66667	0.51813
	Cl_B	0.33333	0.66667	0.61023
	P	0.66667	0.33333	0.48742
	Cl_P	0.66667	0.33333	0.38423
Cl–BP–Br	B	0.33333	0.66667	0.51479
	Cl	0.33333	0.66667	0.60661
	P	0.66667	0.33333	0.48430
	Br	0.66667	0.33333	0.37430
Br–BP–Cl	Br	0.33333	0.66667	0.51598
	B	0.33333	0.66667	0.61454
	P	0.66667	0.33333	0.48624
	Cl	0.66667	0.33333	0.38324
Br–BP–Br	B	0.33333	0.66667	0.51834
	Br_B	0.33333	0.66667	0.62014
	P	0.66667	0.33333	0.48762
	Br_P	0.66667	0.33333	0.37390

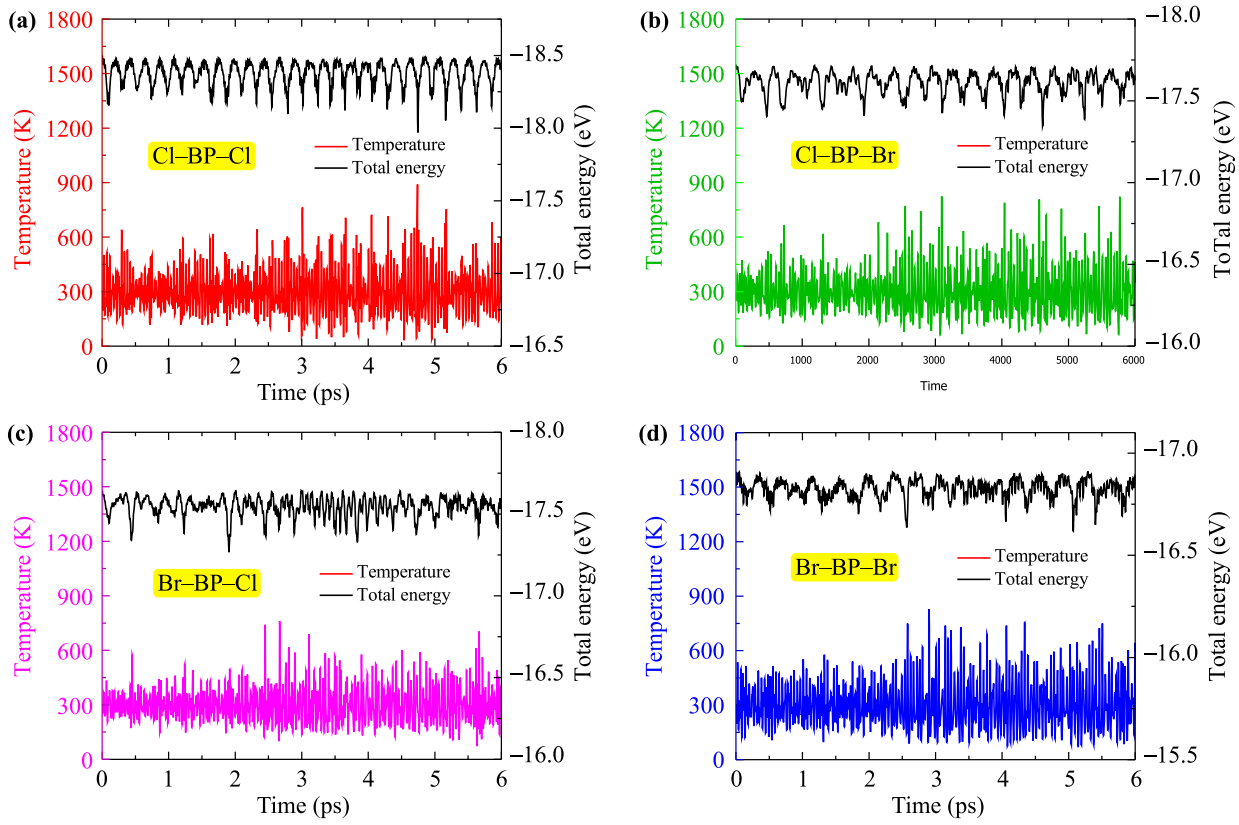

Fig. S1. AIMD simulations for the fluctuations of temperature and total energy as functions of time of the functionalized boron phosphide with Br and Cl: (a) Cl–BP–Cl, (b) Cl–BP–Br, (c) Br–BP–Cl, and (d) Br–BP–Br.

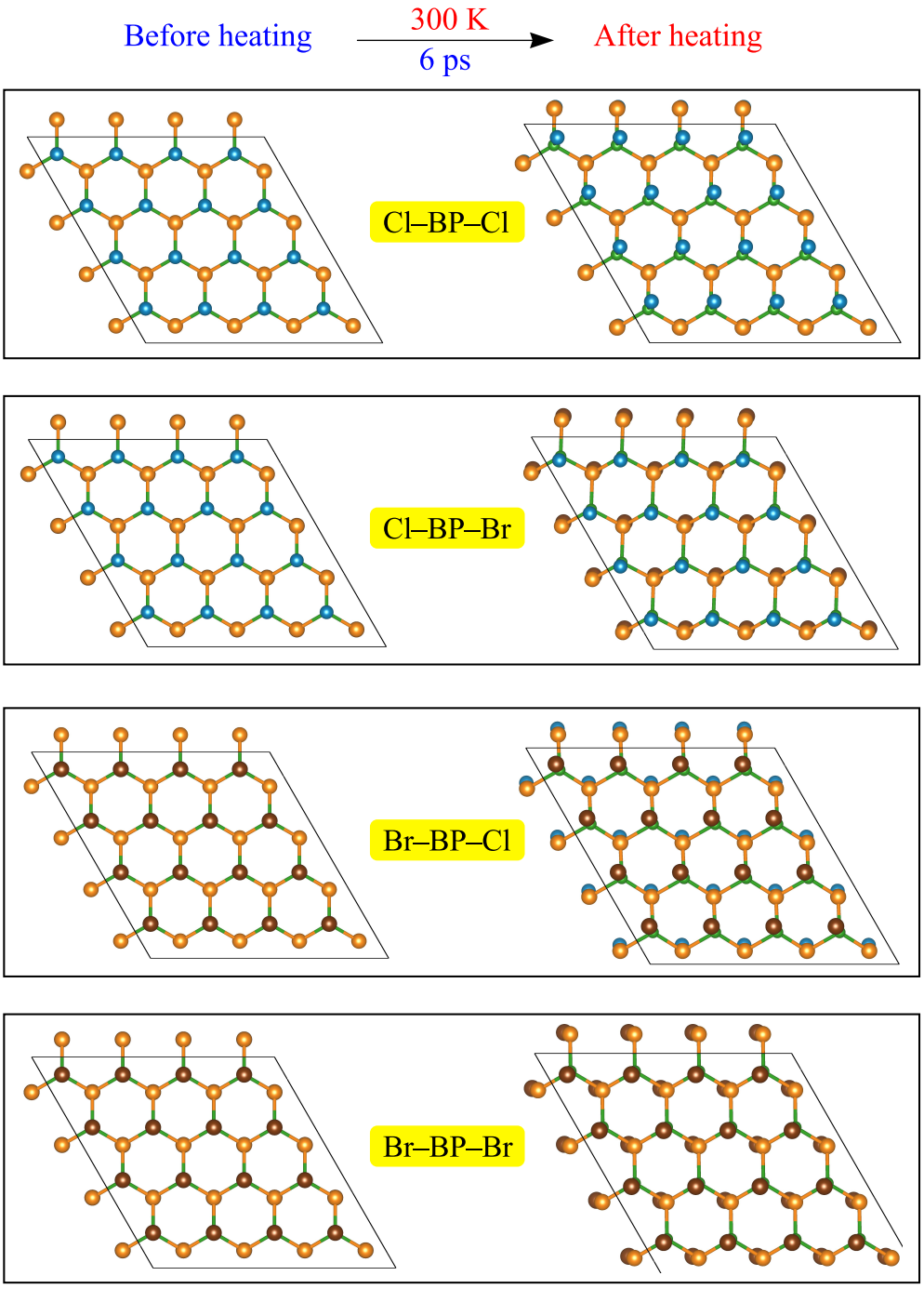

Fig. S2. Snapshots of the atomic structures of the surface-functionalized BP before (left panel) and after (right panel) heat treatment at 300 K within 6 ps. Green, yellow, brown, and blue balls refer to the B, P, Cl, and Br atoms, respectively.