Supplementary Information

Sodium Bismuth Dichalcogenides: Candidates of Ferroelectric High-mobility Semiconductors for Multifunctional Applications

Tingting Zhong,[1] Minghu Pan,[1] Guoying Gao,[1] Huahua Fu,[1] Menghao Wu,[1]* Jun-Ming Liu[2]

[1]School of Physics, Huazhong University of Science and Technology, Wuhan, Hubei 430074, China

[2]Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, China

Table S1. Fitted parameters A, B, C in Landau-Ginzburg expansion.

	A	B	C
$NaBiS_2$	**-5.97**	**-29.27**	**771.26**
$NaBiSe_2$	**-5.26**	**-98.23**	**1223.03**

Table S2. Calculated effective mass m * (with m0 being the static electron mass), deformation potential E_l, elastic modulus C and carrier mobility u along the x and y directions.

	m_x^*/m_0	m_y^*/m_0	E_{lx} (eV)	E_{ly}	C_{x_3D} (J • m^{-3})	C_{y_3D}	u_{x_3D} (10^3 cm^2 • V^{-1} • s^{-1})	u_{y_3D}
3% biaxial strain $NaBiS_2$	0.21	0.38	-7.47	-4.52	0.56×10^{11}	0.50×10^{11}	3.04	1.68
$Na_{0.5}K_{0.5}BiS_2$	0.37	0.42	-6.37	-3.93	0.38×10^{11}	0.33×10^{11}	0.69	1.14
$NaBi_{0.75}V_{0.25}S_2$	0.26	0.43	-4.61	-6.11	0.44×10^{11}	0.36×10^{11}	3.68	0.49

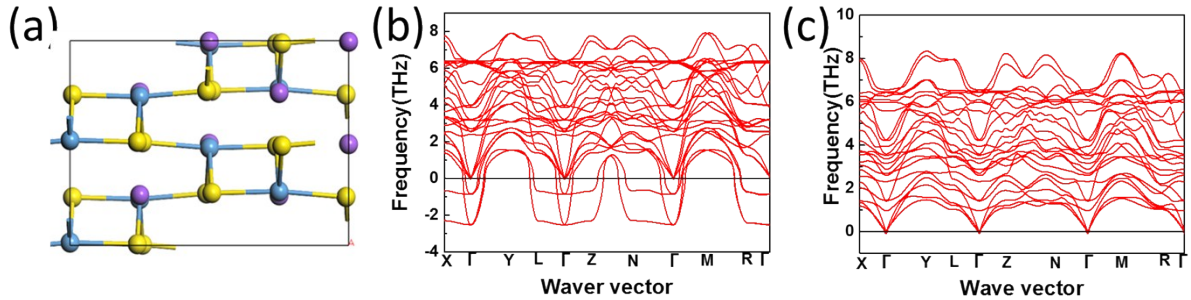

Figure S1. (a)Antiferroelectric configuration of $NaBiS_2$. Phonon dispersion of (b)paraelectric and (c)FE phase for $NaBiS_2$ calculated by using Phonopy.

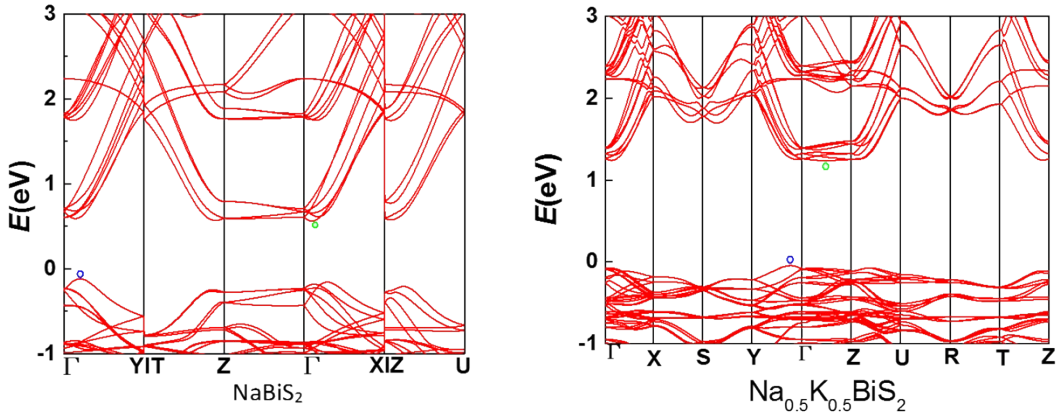

Figure S2. Bandstructures of $NaBiS_2$ and $Na_{0.5}K_{0.5}BiS_2$ by using PBE+SOC.

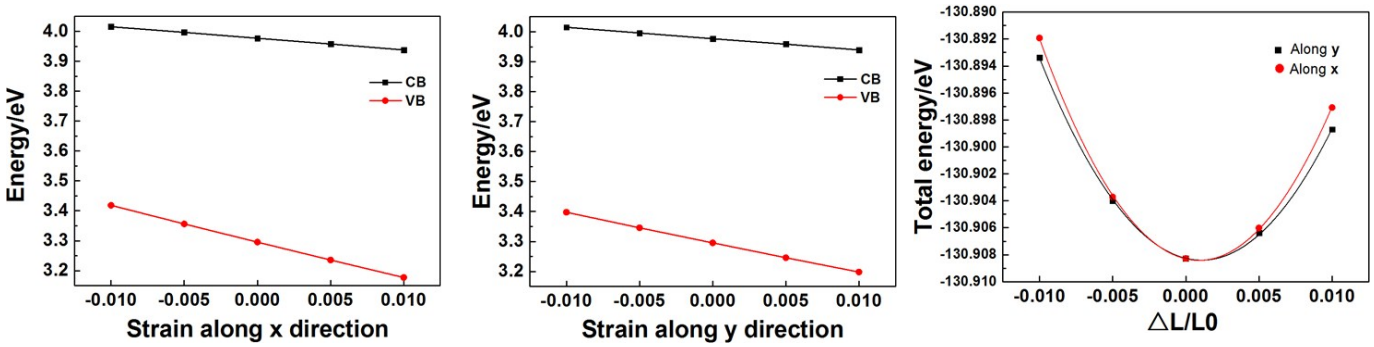

Figure S3. E_1 obtained by linearly fitting the energy shift of the band energy position (CBM and VBM) with respect to a small lattice strain along the –x (left) and –y (middle) direction, and C_{111} calculated based on the quadratic relation between the total energy and lattice dilations under strain (right).

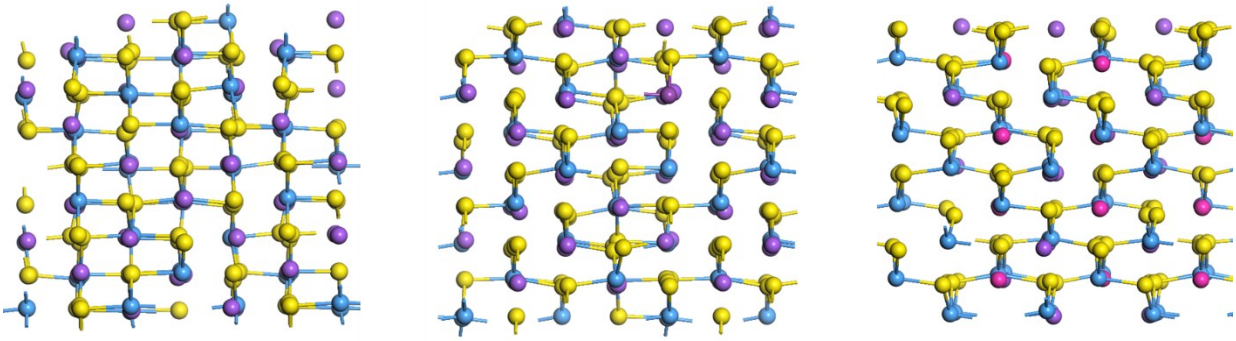

Figure S4. Snapshot of the equilibrium structures at 300K for pristine $NaBiS_2$ (left), $NaBiS_2$ upon a 3% biaxial strain at xy plane (middle), and $Na_{0.5}K_{0.5}BiS_2$ (right) at the end of 10ps of ab initio MD simulation with a canonical ensemble (time step is set as 1fs).