附录

表 S1　c-Li_3N 和 c-Na_3P 材料中各原子轨道对价带顶(VBM)和导带底(CBM)上电子态的贡献

Tab. S1　The contribution of atomic orbitals of c-Li_3N and c-Na_3P to the electronic states at the valence-band maximum (VBM) and the conduction-band minimum (CBM)

	Li/Na				N/P			
	s	p_x	p_y	p_z	s	p_x	p_y	p_z
c-Li_3N (VBM)	0	0	0	0.173	0	0	0	0.459
c-Li_3N (CBM)	0.056	0.019	0.005	0	0.039	0.200	0.010	0
c-Na_3P (VBM)	0	0.000	0.011	0.029	0.000	0.002	0.081	0.203
c-Na_3P (CBM)	0.069	0.000	0	0	0.062	0	0	0