Supplementary Information for

On the ferroelectricity in wurtzite materials

Zijian Zhou,[1] Kan-Hao Xue,[1,2,*] Jinhai Huang,[1] Heng Yu,[1] Shengxin Yang,[1] Shujuan Liu,[2] Yiqun Wang,[2] Xiangshui Miao[1,2]

[1]School of Integrated Circuits, Huazhong University of Science and Technology, Wuhan 430074, China.

[2]Hubei Yangtze Laboratory, Wuhan 430205, China

*Corresponding author: xkh@hust.edu.cn

Table S1. Bader charge transfer of all IIIA-V and IIB-VI compounds arranged in the WZ structure.

IIIA-V	Bader Charge	IIB-VI	Bader Charge
BN	2.13686	**ZnO**	1.22337
BP	0.40578	**ZnS**	0.87372
BAs	0.04533	**ZnSe**	0.73602
AlN	2.36078	**ZnTe**	0.5076
AlP	2.02543	**CdO**	1.12944
AlAs	1.88763	**CdS**	0.84061
AlSb	1.57657	**CdSe**	0.70704
GaN	1.51541	**CdTe**	0.51769
GaP	0.81868		
GaAs	0.63654		
GaSb	0.30898		
InN	1.39908		
InP	0.85796		
InAs	0.72561		
InSb	0.44502		

Table S2. The integral Crystal Orbital Bond Index (ICOBI) of WZ-ZnO, WZ-ZnS, WZ-GaN, and WZ-GaAs.

	GGA	**DFT+U ($U = 10$ eV)**
ZnO	0.18587	0.18415
ZnS	0.10664	0.10372
GaN	0.65582	0.62527
GaAs	0.82791	0.81132

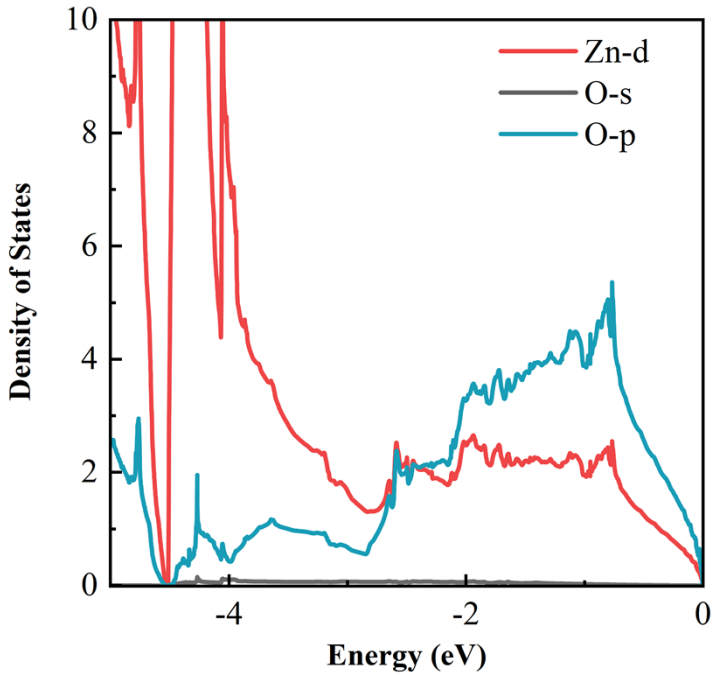

Figure S1. PDOS of WZ-ZnO near E_f.