The magnetism and electronic structures of bilayer Bismuth (Stannum) films on monolayer CrI_3 ($CrBr_3$) interface

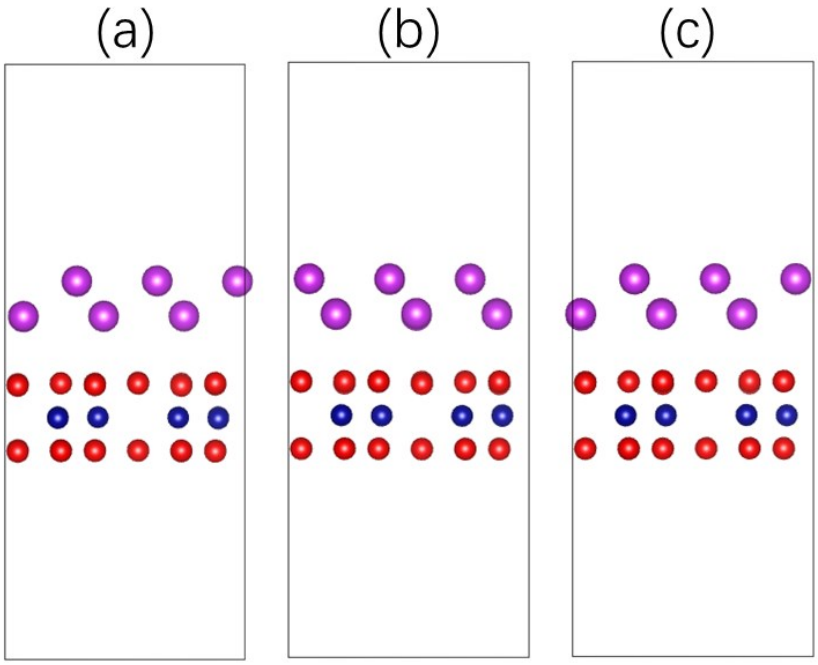
Li Chen[a,b*], Chuan Jiang[c*], Maoyong Yang[a], Tao Hu[a], Yan Meng[a], Jie Lei[a], Mingjian Zhang[a]

[a]*School of Electronic and Information Engineering (Department of Physics), Qilu University of Technology, Jinan 250353, China*

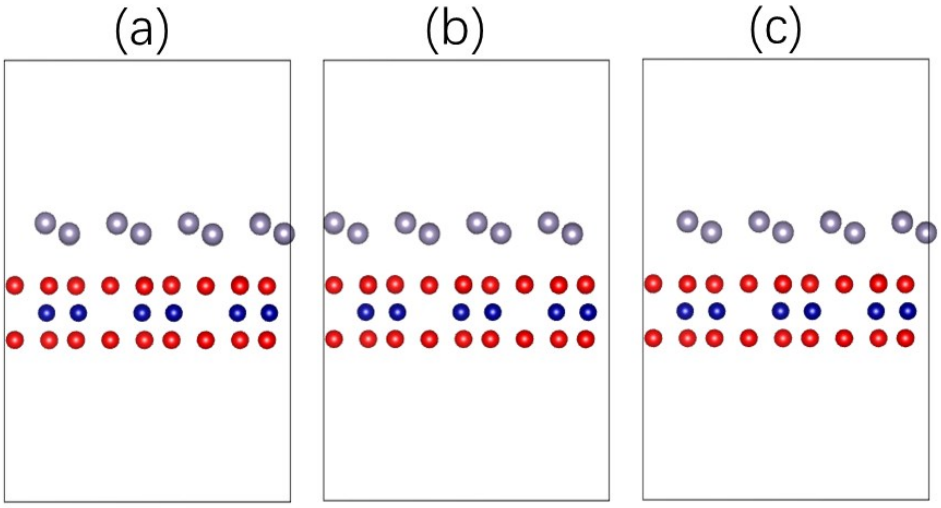
[b] *Institute of Condensed Matter Physics, Linyi University, Shandong 276000, China*

[c] *Department of Data Acquisition, National Instruments, Shanghai 201204, China*

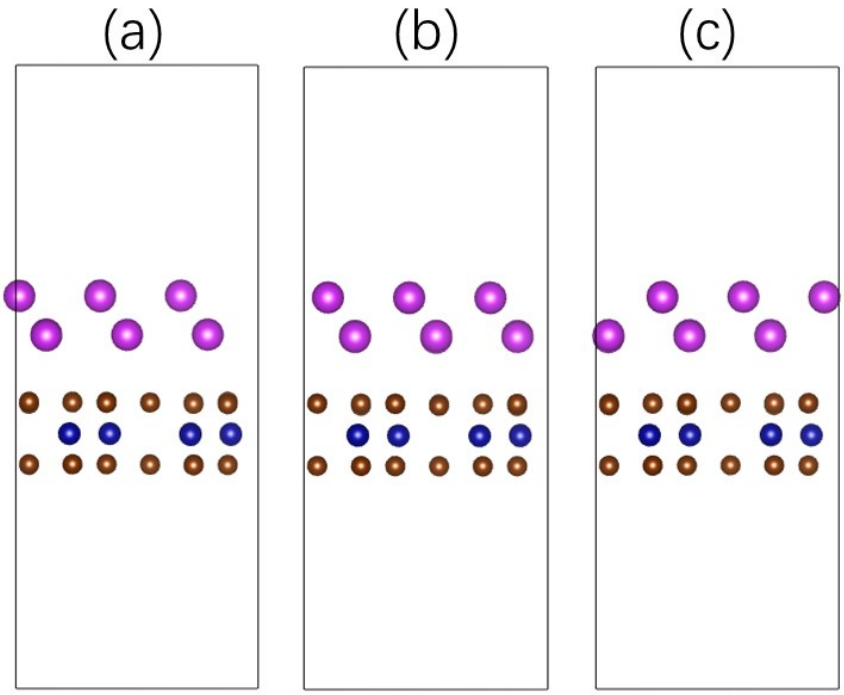
Correspondence: chenli@qlu.edu.cn(L.C.); jiangcn@mail.uc.edu(C.J.)



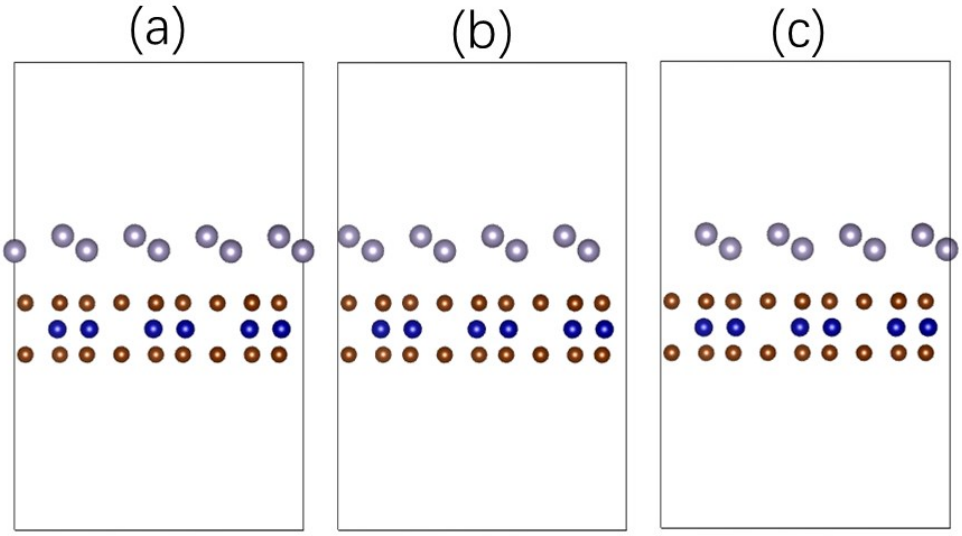
Supplementary materials Figure s1. (Color online). Side view of the interfacial atomic structure of 1BL-Bi on 1ML-CrI_3. (a) one Bi atom at bridge site of I atoms; (b) one Bi atom at hollow site of I atoms; (c) one Bi atom at top site of I atoms. Magenta, blue and red balls represent Bi, Cr and I atoms, respectively.



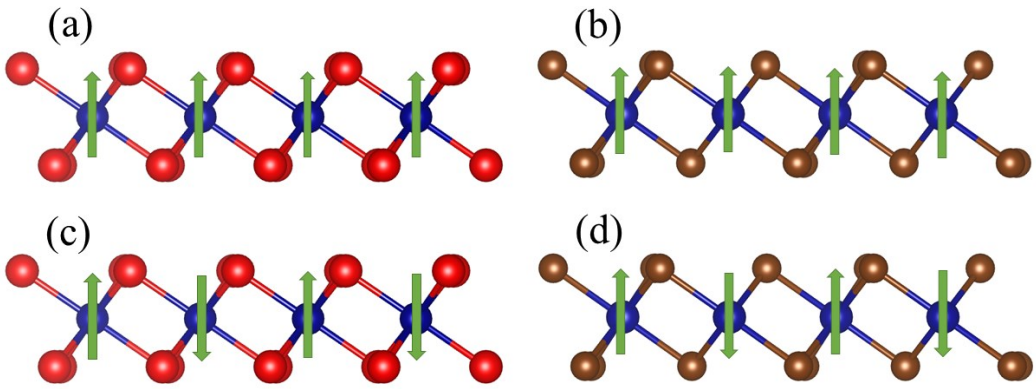
Supplementary materials Figure s2. (Color online). Side view of the interfacial atomic structure of 1BL-Sn on 1ML-CrI_3. (a) one Sn atom at bridge site of I atoms; (b) one Sn atom at hollow site of I atoms; (c) one Sn atom at top site of I atoms. Gray, blue and red balls represent Sn, Cr and I atoms, respectively.



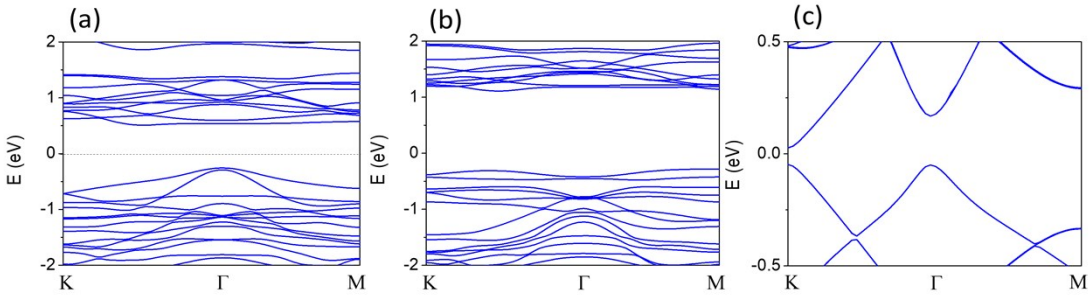
Supplementary materials Figure s3. (Color online). Side view of the interfacial atomic structure of 1BL-Bi on 1ML-$CrBr_3$. (a) one Bi atom at bridge site of Br atoms; (b) one Bi atom at hollow site of Br atoms; (c) one Bi atom at top site of Br atoms. Magenta, blue and wine balls represent Bi, Cr and Br atoms, respectively.



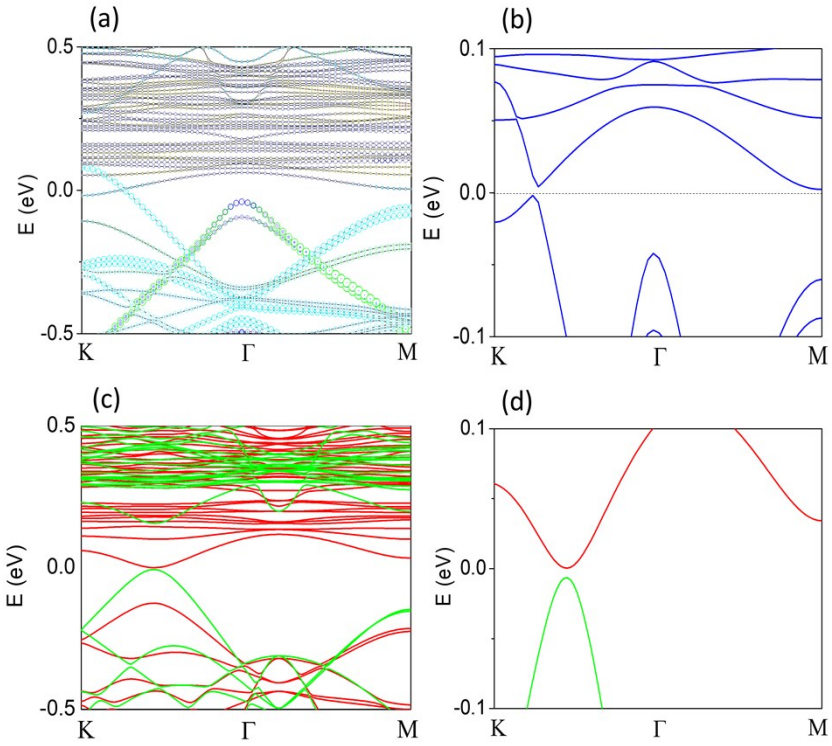
Supplementary materials Figure s4. (Color online). Side view of the interfacial atomic structure of 1BL-Sn on 1ML-$CrBr_3$. (a) one Sn atom at bridge site of Br atoms; (b) one Sn atom at hollow site of Br atoms; (c) one Sn atom at top site of Br atoms. Magenta, blue and wine balls represent Sn, Cr and Br atoms, respectively.



Supplementary materials Figure s5. (Color online) The ferromagnetic (FM) configuration with the same out-of-plane spin orientation. (a) for CrI_3 and (b) for $CrBr_3$. The AFM configuration with antiparallel spin orientation between nearest neighbors. (c) for CrI_3 and (d) for $CrBr_3$.



Supplementary materials Figure s6. (Color online) Band structures long K-Γ-M directions with SOC (a) for ML-CrI_3, (b) For ML-$CrBr_3$, and (c) For BL-Sn film.



Supplementary materials Figure s7. (Color online) (a) Band structures without U correction for BL-Sn/ML-$CrBr_3$ interface system. The red, green, blue, cyan, magenta, yellow, dark yellow, navy and purple lines on the bands illustrate the contribution of s, p_x, p_y, p_z, d_{xy}, d_{yz},d_{z2}, d_{xz} and d_{x2-y2} states, respectively; (b) Enlarge view of band structure for interfacial Sn/$CrBr_3$ system; (c) Band structure for interfacial Sn/$CrBr_3$ system with magnetic polarization and without SOC and U correction; (d) Enlarge view of band structure (c). Here red and green color shows the contribution of up spin and down spin, respectively.