

Drumhead Surface State Promoted Hydrogen Evolution Reaction in Type-II Nodal-Line Topological Catalyst Mg_3Bi_2

Min Zhao ¹, Weizhen Meng ^{2*}, Lirong Wang ¹, Zeqing He ¹, Lei Jin ¹, Ying Liu ¹,
Xuefang Dai ¹, Xiaoming Zhang ^{1*}, Hongshi Li ^{1*}, and Guodong Liu ^{1*}

1. State Key Laboratory of Reliability and Intelligence of Electrical Equipment, and School of Materials Science and Engineering, Hebei University of Technology, Tianjin, 300130, China.

2. College of Physics, Hebei Key Laboratory of Photo physics Research and Application, Hebei Normal University, Shijiazhuang, 050024, China.

E-mail of corresponding authors: meng199608@126.com; zhangxiaoming87@hebut.edu.cn;
ish82@126.com; gdlou1978@126.com

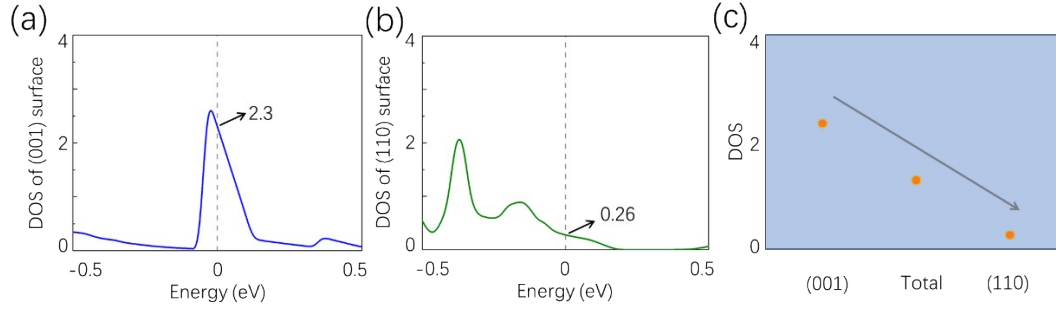


Figure S 1 (a) - (c) Electronic density of states of (001), (110) and bulk bands near Fermi level in Mg_3Bi_2 with Kagome lattice, respectively.

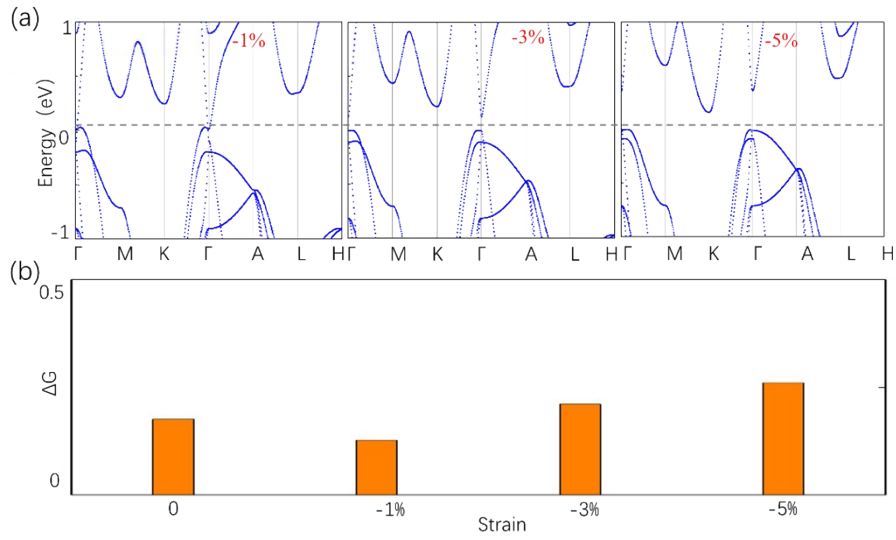


Figure S2. (a) and (b) The electronic band structures and ΔG_H under different strains, respectively.

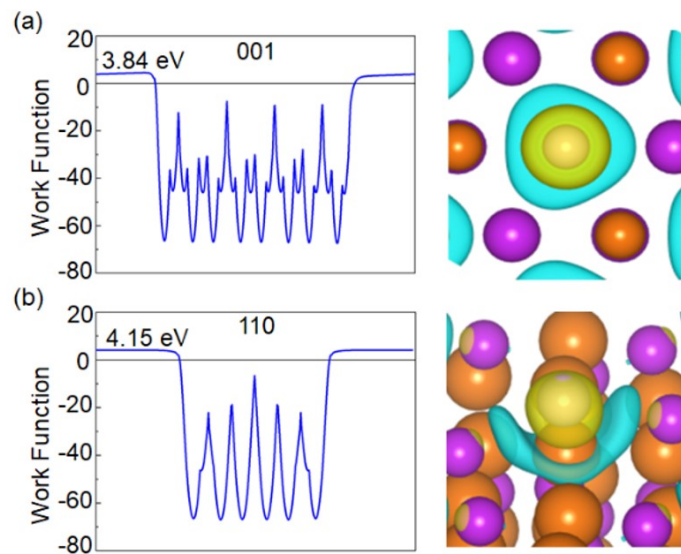


Figure S 3 (a) and (b). The work function and charge differential density of Mg_3Bi_2 on (001) and (110) surfaces, respectively.

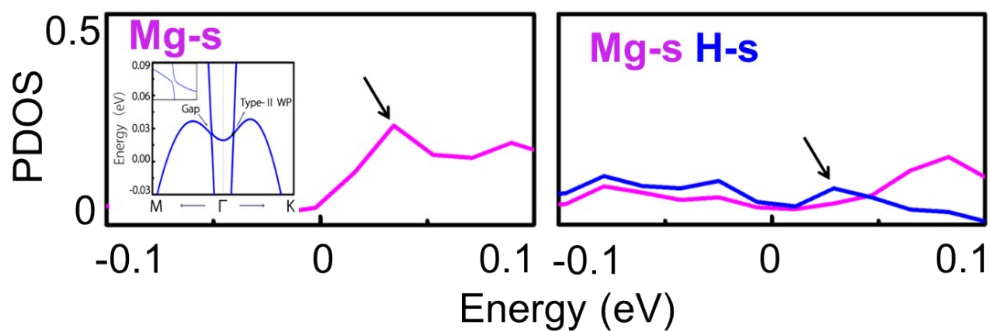


Figure S 4. Projected DOS of the active Mg-s orbital of Mg_3Bi_2 catalyst before and after interacting with the H intermediate

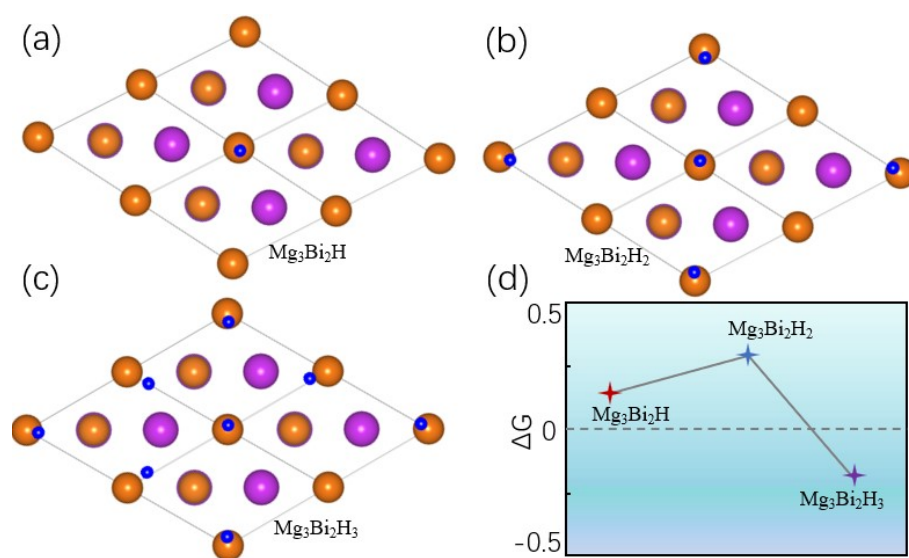


Figure S 5 (a) - (c) The optimized supercell structure of $\text{Mg}_3\text{Bi}_2\text{H}$, $\text{Mg}_3\text{Bi}_2\text{H}_2$, $\text{Mg}_3\text{Bi}_2\text{H}_3$, respectively. (d) Gibbs free energy of Mg_3Bi_2 under different hydrogen coverages.