Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Adsorption and dissociation of H2O molecules on the topological insulator surface, Bi_2Se_3 (111)[1] EUN-HA SHIN, HANCHUL KIM, Sookmyung Women's University — Three-dimensional strong topological insulators (TIs) such as Bi_2Se_3, Bi_2Te_3 and Bi_2Sb_3 are intriguing for their surface metallicity in contrast to the insulating bulk. The metallic surface states of TI are known to be topologically protected and robust for impurities and disorders. In this work, we report first-principles calculations on the adsorption and dissociation of H_2O molecules on Bi_2Se_3 (111) to understand the chemical reactivity and the effect of oxidation on the surface metallicity. On the pristine (111) surface, H_2O molecule is found to chemisorb on a subsurface Bi atom and form two additional hydrogen bonds with neighboring surface Se atoms. The adsorbed H_2O molecule can be dissociated into a hydroxyl (OH) and H. The dissociated OH takes a surface Se site, and pushes up the Se atom that is bonded with the dissociated H. We examined a subsequent dissociation reaction of OH. The final reaction products are a substitutional O (O_{Se}) and an H_2Se molecule floating in the vacuum. By examining the electronic structure, we found that the chemisorbed OH induces n-type doping. On the other hand, the O_{Se} and the adsorbed H_2O result in p-type doping. Throughout the whole chemical processes studied, the metallic surface state remains intact.

[1]This work was supported by a National Research Foundation of Korea grant (No. 20100012231) and the EDISON program (No. 2012M3C1A6035684) funded by the Korea government(MEST), and by the Supercomputing Center at KISTI (No. KSC-2014-C3-042).

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Date submitted: 14 Nov 2014 Electronic form version 1.4