

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Transition metal dichalcogenides as a catalyst for hydrogen-evolution reaction JUN-HO LEE, YOUNG-WOO SON, Korea Inst for Advanced Study, JINBONG SEOK, HEEJUN YANG, Department of Energy Science and IBS Center for Integrated Nanostructure Physics, Institute for Basic Science, Sungkyunkwan University — Hydrogen evolution using electrochemical reaction of water with specific catalysts has been considered as next-generation energy resources. The best-well known and most productive electrochemical catalyst is platinum. However, there has been a continuous struggle to replace the precious Pt-based catalysts by inexpensive and earth-abundant materials such as transition metal dichalcogenides (TMDs). We investigated catalytic performances of various TMDs for hydrogen-evolution reaction (HER) by using first-principles density functional theory calculation. We calculate Gibbs free energy, most widely used descriptor of catalytic activity, of hydrogen atom on TMDs and analyze an origin of significant performance of HER.

Jun-Ho Lee
Korea Inst for Advanced Study

Date submitted: 05 Nov 2015

Electronic form version 1.4