

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Combinatorial Search of Hydrogen Catalysts Based on Transition Metal Embedded Graphitic Carbons WOON IH CHOI, BRANDON WOOD, ERIC SCHWEGLER, TADASHI OGITSU, Lawrence Livermore National Laboratory, QUANTUM SIMULATION GROUP TEAM — To find right d-orbital configuration for hydrogen catalyst among embedded transition metal (TM) atoms into the lattice of graphene, we performed high-throughput computational search out of 300 combinatorial material pools. Theoretical criteria, so called descriptors regarding material stability and catalytic activity are considered and we were able to narrow down to ten materials for hydrogen evolution, two for hydrogen oxidation reaction. Since catalytically active sites are isolated to single TM atom, Volmer-Kubas type of new reaction pathway is expected for hydrogen evolution. Earth-abundant element Mo, bulk form of which doesn't show good catalytic activity at all, turns into catalytically active site as it is dispersed atomically and its d-orbitals splits by the symmetry of local coordination at the binding sites.

Wooni Choi
Lawrence Livermore National Laboratory

Date submitted: 30 Oct 2014

Electronic form version 1.4