Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Enhanced Dihydrogen-Metal Interaction in Transition Metal Exposed Paddle-Wheel Frameworks YONG-HYUN KIM, KAIST, JOONGOO KANG, SU-HUAI WEI, National Renewable Energy Laboratory, JI HYUN BAK, KAIST — The experimentally observed enhancement of hydrogen adsorption in Cu_2-tetracarboxylate paddle-wheel frameworks is investigated by first-principles density-functional theory calculations [1]. We reveal that the puzzling enhancement is due to the effective orbital coupling between the occupied H_2 σ and the unoccupied Cu $4s$-derived states. The nontrivial dihydrogen-metal σs interaction is enabled by a strong localization of the Cu $4s$ orbital after hybridizing with the neighboring oxygen $2p$ orbitals. Based on this understanding, we predict that the dihydrogen-metal interaction can be further increased by alloying Cu with s-orbital element Zn or Mg. We will also discuss on the enhanced dihydrogen adsorption on other $3d$-transition-metal paddle wheel frameworks.

[1] Y.-H. Kim, J. Kang, and S.-H. Wei, Phys. Rev. Lett., in press (2010).

Yong-Hyun Kim
KAIST

Date submitted: 23 Dec 2010 Electronic form version 1.4