Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First-principles study of water on Cu (110) surface JUN REN, SHENG MENG — The persistent demand for cheaper and high efficient catalysts in industrial chemical synthesis, such as ammonia, and in novel energy applications, hydrogen generation and purification in fuel cells motivated us to study the fundamental interaction involved in water-Cu system, with an intension to examine Cu as a possible competitive candidate for cheaper catalysts. Water structure and dissociation kinetics on a model open metal surface: Cu (110), have been investigated in detail based on first-principles electronic structure calculations. We revealed that in both monomer and overlayer forms, water adsorbs molecularly, with a high tendency for diffusion and/or desorption rather than dissociation on clean surfaces at low temperature. With the increase of the water coverage on the Cu (110) surface, the H-bond pattern lowers the dissociation barrier efficiently. More importantly, if the water molecule is dissociated, the hydrogen atoms can diffuse freely along the [110] direction, which is very useful in the hydrogen collection. In addition, we extended to study water on other noble metal (110) surfaces. The result confirms that Cu (110) is the borderline between intact and dissociative adsorption, differing in energy by only 0.08 eV. This may lead to promising applications in hydrogen generation and fuel cells.

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Date submitted: 21 Nov 2008 Electronic form version 1.4