

Abstract Submitted  
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**Comparative analysis of density functional theory for hydrogen adsorption on metalloporphyrin incorporated graphenes<sup>1</sup>** YUNGOK IHM, Univ of Tennessee, Knoxville, CHANGWON PARK, ORNL, YONG-HYUN KIM, KAIST, Korea, MINA YOON, ORNL, ORNL-UTK TEAM, KAIST COLLABORATION — Porphyrins are often found in nature. The center of the molecules is chemically highly active, thus they can accommodate various metals with high structural stability. A recent study using density functional theory (DFT) suggests that metal incorporated porphyrins can store H<sub>2</sub> in significant amounts at the uniformly distributed metal centers, indicating their great potential as a material for hydrogen storage. In this work, we evaluate the performance of DFT exchange-correlation (XC) functionals to describe the properties of hydrogen adsorption on porphyrin-incorporated graphenes (PIG). We studied PIGs doped with different metals (Mg, Ca, Zn, Ti, V) using various XC functionals, ranging from LDA to van der Waals corrected functionals. Metals interacting with hydrogen through chemical binding, dominated by the Cubas mechanism, have a hydrogen binding strength with much stronger dependence on the XC functional than van der Waals systems. The specific shape of the hydrogen energy potential near metal centers is important in determining the thermodynamic stabilities of the hydrogen adsorption and desorption mechanism. The insights obtained in this work should be useful also when applying DFT methods to more generalized adsorption systems.

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