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WITHDRAWN Density Functional Theory Study of Hydrogen on Metal Oxide and Insulator Surfaces

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Hydrogen molecule is being promoted as an environmentally clean energy source of the future. In order to use hydrogen as a source of energy, infrastructures have to be built. These infrastructures are efficient processes for hydrogen extraction, and efficient processes and materials for hydrogen storage. The major problem facing the use of hydrogen as a clean source of energy is the storage of liquid hydrogen. Hydrogen fuel can be concentrated into a small volume and store it in fuel tanks. The concentration of hydrogen can be done simply by cooling the hydrogen to an extremely low temperature or by compressing it under very high pressure as liquid. The concentrated normal mixture consist 25% *p*-H2, 75 % *o*-H2 and after hours of storage, about 40 % of the original content of the tank evaporates. The reason of this evaporation is the spontaneous conversion of orthohydrogen (*o*-H2) to parahydrogen (*p*-H2) over a period of time. This conversion is releasing enough heat to evaporate most of the liquid hydrogen and yield the explosion of the tank storage. In order to overcome this problem and limit the boil-off to low levels, the tank most be fill with a liquid hydrogen that has already been converted to a mixture close to 100 % *p*-H2. Special procedures are needed to maintain the composition (proportion) of the two types of hydrogen molecules (*o*-H2) and parahydrogen (*p*-H2) to be 100 % *p*-H2.

In this presentation we will discuss the results of DFT methods of hydrogen molecule physisorbed on SrTiO3, Fe(OH)3 and MgO(001) surfaces. Energies, orbitals, positions and vibration frequencies of H2 molecule on these surfaces are calculated. Our results show that H2 molecules can physisorbed on these surfaces and that these surfaces induce o–p conversation of H2. The effect of molecular orientations and positions of H2 molecules on the catalysts surface on the *o-p* H2 conversion yield will be presented.

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