An effective way of enhancing hydrogen storage on adsorbent materials is provided by the hydrogen spill-over mechanism, although there is no general consensus to date to satisfactorily explain the mechanism. In this work a possible reaction path to explain the hydrogen adsorption is shown. Density-functional calculations were used to study the dissociation of molecular hydrogen near to a stressed region as consequence of chemisorbed hydrogen on the graphenenitrogen surface. We found that, as a result of the buckling induced by the chemisorbed hydrogen, the dissociation barrier of molecular hydrogen is lowered 0.84 eV. The chemisorbed hydrogen is the final state in the spill-over mechanism on graphene-nitrogen decorated with palladium clusters. This effect helps to create hydrogen nanoislands that may change the diffusion and detrapping of H. An electronic structure analysis suggests that the systems occasionally behave as metallic or semiconductor.

**Keywords:** spill-over, chemisorbed hydrogen, buckling

**Acknowledgment:**

F. Martínez-Farias. was partialy supported by grant UAEHPTC764, DSA/5116/178021. Part of this work was performed at the CNMS wich is a US DOE Office of Science User Facility at ORNL Supported under contract no. DE-AC05-00OR22725.

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