Department of Physics  
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Departmental Seminar

Metal decorated 2D-C$_2$N as promising hydrogen storage materials

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**Date:** 16.11.2018 **Time:** 3:10 pm  
**Venue:** Seminar Hall (GF), Department of Physics, CUTN.

**Abstract**

In an effort to overcome the energy demand and related issues, a great deal of attention has been focused on search for alternative clean energy resources. Hydrogen has been considered for many years as a clean energy carrier because of its abundance, efficiency, and environmental friendliness. [1] However, it is a highly challenging practical issue to store hydrogen in a safe and efficient way. For mobile applications, hydrogen storage materials should store hydrogen reversibly with high gravimetric densities. Based on this, many hydrogen storage materials such as metal hydrides, complex hydrides, and nano materials has been considered. However, the disadvantages of these materials such as high decomposition temperatures, insufficient storage capacity, poor sorption kinetics and reversibility still remain unsolved. Among the several hydrogen storage materials, a newly synthesized 2D nitrogenated holey graphene have paved the way for the development of next-generation promising material for reversible hydrogen storage with a high capacity owing to its light weight, inexpensive, and large surface to volume ratio. [2] It was also found that the interaction between H$_2$ and the neutral C$_2$N is very weak with the adsorption energy of only 0.06 eV. At ambient conditions, the H$_2$ binding energy with the host material should lie within 0.2–0.6 eV to use it as hydrogen storage media. It was reported that the decoration of the carbonaceous nano materials with metal atoms could significantly improve the H$_2$ adsorption energy. Very recently, it was found that Li decoration in C$_2$N monolayer improved the H$_2$ adsorption energy and store hydrogen reversibly with high capacity. [3] In our studies, we have decorated Mg in C$_2$N monolayer since Mg is cheap and abundant element that can hold more H atoms per metal ion than Li and currently investigating its hydrogen storage properties. In this presentation, I will explain the basics of hydrogen storage and how the metal decoration will improve the hydrogen storage properties of C$_2$N monolayer. the full DNA model. Energy localization in the form of discrete breathers and solitons via modulational instability will be addressed in this seminar.

**References:**  

**All are welcome**

Seminar Coordinators  
Head of the Department