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Departmental Seminar

Metal decorated 2D-C_2N 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_2N 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_2N monolayer improved the H_2 adsorption energy and store hydrogen reversibly with high capacity. [3] In our studies, we have decorated Mg in C_2N 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_2N 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:

[1] Gielen. D, Boshell. F, Saygin. D, Nat. Mater 2016, 15, 117-120.
[2] Qin, Cui Gangqiang, Yun Qianyi, Sun Baofeng, Du Lixian, Sun Aijun, Qiao, Int. J. Hydrogen Energy 2018, 43, 9895-9901.
[3] Arqum Hashmi, M. Umar Farooq, Imran Khan, Jicheol Son and Jisang Hong, Mater. Chem. A 2017, 5, 2821.

All are welcome

Seminar Coordinators Head of the Department