Contribution ID: **408** Type: **Poster**

First-principles study of H_2 adsorption on two-dimenstional C_2N sheet

Wednesday 24 May 2017 15:45 (15 minutes)

First-principles calculations based on density functional theory (DFT) have been performed to study the adsorption of molecular H_2 on the graphene-like material C_2N. The possible adsorption sites on top of bonds, on carbon atom and nitrogen atom and the center of C-C hexagon and the C-N hexagon are considered. The adsorption energies for each site are calculated and are found to be in the physisorption regime. We find that the most favorable site of H_2 is above the center of C-N hexagon. In addition, we demonstrate that inclusion of the Van der Waals interactions through the DFT-D2 method via the generalized gradient approximation (GGA) functional gives the consistent trend of H_2 adsorption with that obtained via the local-density approximation (LDA) functional. The effects of Van der Waals interactions on the adsorption energies and equilibrium distance between H_2 and C_2N sheet are discussed.

Primary author: Mr NETRATTANA, Pongdet (Department of Physics, Faculty of Science, Kasetsart University)

Co-author: REUNCHAN, Pakpoom (Kasetsart University)

Presenter: Mr NETRATTANA, Pongdet (Department of Physics, Faculty of Science, Kasetsart University)

Session Classification: Poster Presentation I

Track Classification: Nanoscale Physics and Nanotechnology