Contribution ID: **758** Type: **Poster**

Stability and physical properties of Mn-doped ZnO monolayer

Monday 21 May 2018 18:30 (15 minutes)

Recently, monolayer of ZnO has successfully been synthesized on graphene. It leads to a new class of 2D oxide materials which have many promising properties such as high optical transparency, hazard gas capture etc. To improve to use in a spintronic application, Mn is doped into ZnO by many previous studies. Here, this study aims at investigating stability, electronic and magnetic properties and CO absorbance of ZnO monolayer doped with Mn atom by means of *ab initio* calculation. Mn atom is substituted at a cation Zn position of the ZnO monolayer with the cell sizes of 2×2, 2×4 and 4×4 which correspond to 50 and 25, 12.5, and 6.25 Zn-at%Mn, respectively. The finding shows that all Mn-doped ZnO monolayers are stable in the thermodynamic stability and the binding energy decreases with increasing atomic percentage of Mn atom. The Mn-doped ZnO monolayer exhibits a ferromagnetic semiconductor as mainly due to the strong 2p-O and 3d-Mn mixing orbital. The band gap of undoped ZnO monolayer is larger than the band gap of wurtzite ZnO about 1 eV which is in agreement with experimental result (˜0.7 eV). We also find that the band gap of Mn-doped ZnO is reduced by number of Mn atoms, this situation might be influenced by the spin polarization of 3d-Mn state below the Fermi level. The distortion of O atoms surrounding a Mn atom is occurred because the nature of Mn is a better oxidant than Zn atom. Moreover, Mn atom tend to attract C atom in CO molecule but extrude O atom. These results might be potentially useful for the spintronic application, the development of magnetic 2D oxide materials, and CO absorbance.

Primary authors: ROONGRUANGSAK, Thanwarat (Mahidol Wittayanusorn School); YUBONKET, Kitsanakorn (Mahidol Wittayanusorn school); AUPPAKHUN, La-orrat (Mahidol Wittayanusorn School)

Co-author: KOTMOOL, Komslip Kotmool

Presenters: ROONGRUANGSAK, Thanwarat (Mahidol Wittayanusorn School); YUBONKET, Kitsanakorn (Mahidol Wittayanusorn school); AUPPAKHUN, La-orrat (Mahidol Wittayanusorn School)

Session Classification: A05: Nanoscale and Surface (Poster)

Track Classification: Nanoscale Physics and Nanotechnology