



Contribution ID: 29

Type: **Poster Presentation**

Computational study of ZIF with functional groups for CO₂ adsorption.

Tuesday, 26 June 2018 15:00 (2 hours)

Greenhouse gases, Carbon Dioxide in particular, has been a main concern for climate change. Zeolitic Imidazolate Framework (ZIF), a sub class of Metal Organic Framework (MOFs), is a 3-dimensional nanoparticle consisting of metal ion (Zn²⁺) and an organic linker (imidazole) with high chemical and thermal stability. The bond angle between the metal and imidazole has the same 145° angle found in zeolites. These cage like structures are porous and have a high surface area (>1600 m² g⁻¹). The high surface area is advantageous in several applications such as gas storage, gas separation, chemical sensors etc. ZIFs with its organic imidazole counterpart can be easily modified to add or improve functionality of the materials. Additional functional groups on the imidazole linker such as NO₂ groups were found to greatly enhance the CO₂ adsorption capabilities of ZIFs via a ligand exchange process. In this study a series of functional groups on ZIFs were computed with Grand Canonical Monte Carlo (GCMC) simulations by Material Studio to determine whether NO₂, SH, F, Cl, Br, CH₃, OH, NH₂, phenyl and H groups will benefit in improving CO₂ adsorption. Our results show that ZIFs with electron withdrawing groups can greatly enhance CO₂ adsorption and can easily predict which functional group to synthesis experimentally.

Please confirm that you have carefully read the abstract submission instructions under the menu item "Call for Abstracts" (Yes / No)

Yes

Consideration for student awards
Choose one option from those below.
N/A
Hons
MSc
PhD

N/A

Supervisor details
If not a student, type N/A.
Student abstract submission requires supervisor permission: please give their name, institution and email address.

Dr Richard Harris, University of the Free State, HarrisRA@ufs.ac.za

Primary authors: Dr TSAI, Chih-Wei Tsai (University of the Free State); Dr HARRIS, Richard (University of the Free State)

Presenter: Dr TSAI, Chih-Wei Tsai (University of the Free State)

Session Classification: Poster Session 1

Track Classification: Track A - Physics of Condensed Matter and Materials