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Contribution ID: **46** Type: **Invited talk (plenary/keynote)**

Computational chemistry methods in understanding the properties of porous material

Tuesday, 5 December 2017 13:30 (30 minutes)

Intermolecular interactions play a fundamentally important role in the properties of solid materials. For instance, molecules ("guests") are taken up into porous materials ("hosts") as a result of the interactions between these species, while the manner in which they interact has an influence on the sorption ability of the porous material. Several examples from our work will be used to show that calculations performed using the CHPC's computational facility allow us to explain the role that intermolecular interactions play in the unusual sorption properties of various porous compounds. For instance, the interactions between carbon dioxide and a host porous metal-organic framework yield anomalous sorption isotherms.[1] Similarly, intermolecular interactions are responsible for the change in colour of a crystalline porous compound during sorption of certain solvents along an hourglass pattern. Calculations show that the origin of this effect is that the channels in the porous framework are anisotropic, allowing sorption only from particular faces.[2] Calculations also enabled us to understand the changing intermolecular interactions involved in two other porous compounds that could allow the frameworks to undergo large structural changes during sorption and desorption, while still maintaining the integrity of the crystalline nature of the compound. [3]

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[1] Bezuidenhout, C. X.; Smith, V. J.; Bhatt, P. M.; Esterhuysen, C.; Barbour, L. J. Angew. Chem. Int. Ed. 2015, 54, 2079–2083.
[2] Bezuidenhout, C. X.; Esterhuysen, C.; Barbour, L. J. Chem. Commun., 2017, 53, 5618–5621.
[3] Bezuidenhout, C. X.; Smith, V. J.; Esterhuysen, C.; Barbour, L. J. J. Am. Chem. Soc. 2017, 139, 5923–5929.

HPC content

Codes used: Gaussian09, Gaussian16, Materials Studio

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