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Computational chemistry methods in understanding the properties of porous materials

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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 that can be explained by the electrostatic interactions between host and guest.[1] This can be extended to study mixtures of gases, where CO2 and N2 interact differently with the frameworks, leading to non-ideal sorption behaviour that influences the ability of a porous compound to separate CO2 from N2.[2] Molecular dynamics calculations and in combination with simulation of sorption isotherms using the BioVia MaterialsStudio suite available through the CHPC can hence be used to identify materials that will yield superior gas separation compounds.

[1] Bezuidenhout, C. X.; Smith, V. J.; Bhatt, P. M.; Esterhuysen, C.; Barbour, L. J. Angew. Chem. Int. Ed. 2015, 54, 2079–2083.
[2] Costandius, A. J.; Barbour, L. J.; Esterhuysen, C. In preparation.

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