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## COLLOQUIUM

# The role of intermolecular interactions in chemical processes and materials science

Prof Catharine Esterhuysen (Stellenbosch University)

**DATE:** Monday, 29 July 2024 | 16h00–17h00 SAST

**VENUES:**

- Neelsie Cinema, Stellenbosch University
- Online

### ABSTRACT

The most challenging aspect in understanding the properties of materials in the solid state is to identify the role that intermolecular interactions play in their behaviour. 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. So too for catalysts, where the first step in their mechanism of action is the formation of weak interactions between the metal centres and the catalytic substrates. Therefore, the reactivity and selectivity of a catalytic reaction can be tuned by positioning of the substrate relative to the catalyst with the aid of weak intermolecular interactions.

In this presentation, several examples from our work will be used to show that computational methods allow us to explain the role that intermolecular interactions play in a range of chemical processes. In particular, I will focus on how interactions between water, CO<sub>2</sub> and other solvents influence the properties of porous materials, such as allowing the release of water down to temperatures as low as –70°C, anomalous sorption behaviour and solvatochromic effects. The influence of hydrogen and halogen bonding and other weak interactions in catalysis and crystal engineering will also be demonstrated.

### BIOGRAPHY

After completing a PhD in crystallography under the supervision of Gert Kruger at the University of Johannesburg, Catharine Esterhuysen joined Stellenbosch University in 2000. During her studies she developed an interest in computational chemistry, which she was able to develop through Alexander von Humboldt fellowships with Gernot Frenking in Marburg and Tim Clark at Erlangen. Her main research focus is the study of intermolecular interactions, combining her knowledge of computational chemistry and crystallography to explain unusual interactions and their role in the properties of materials. In this context, she has published more than 70 articles in top peer-reviewed journals including *Nature*, *Angewandte Chemie* and *Journal of the American Chemical Society* and has delivered numerous plenary, keynote and invited talks on her work at an international level. She has served on numerous committees and editorial boards, including as president of the South African Crystallographic Society and Associate Editor at *New Journal of Chemistry*.



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