

## S E M I N A R

# From Atoms to Surfaces: DFT Insights into Catalytic and Reactive Surfaces & Interfaces

**Dr David Tshwane** (*NITheCS Associate*)

Friday, 22 August 2025 @ 14h00-15h00 SAST

**Venues:** Online and NITheCS Seminar Room (Room 002 Level 1,  
Merensky building, Stellenbosch University)

### ABSTRACT

Understanding surface adsorption processes at the atomic level is crucial for advancing material design in catalysis, sensing, corrosion resistance, and energy applications. Density Functional Theory (DFT) has emerged as a powerful and widely used computational tool for investigating material surfaces during adsorption phenomena. Employing DFT to model the interaction between various adsorbates and material surfaces, revealing key insights into adsorption energies, charge transfer, surface reactivity, and site selectivity. Through a systematic analysis of surface-adsorbate configurations, the work elucidates the role of surface morphology, electronic states, and functionalization in determining adsorption behavior. The findings contribute to the predictive design of materials with tailored surface properties, enabling improved performance in applications such as hydrogen embrittlement, corrosion and oxidation resistance, heterogeneous catalysis, gas sensing, and surface functionalization.

### BIOGRAPHY



David Tshwane holds a PhD in Physics (2021) and an MSc in Physics (2016), both from the University of Limpopo. He has served as a Senior Researcher at the Council for Scientific and Industrial Research (CSIR) and is an Associate of NITheCS.

An expert in computational modelling and simulation for materials design, discovery, and characterisation, Dr Tshwane has received several awards and honours, including Best PhD Presenter at the SAIP Conference (2019), the CSIR PhD Student Excellence Award (2022), and the NRF Thuthuka Grant (2024). He has represented South Africa at the 9th BRICS Young Scientists Forum and the 7th BRICS Young Innovator Prize, and has been an invited speaker at international events such as the International Aluminium Conference and Exhibition (2022) and key forums in Russia (2024).

Dr Tshwane supervises master's and doctoral students at multiple institutions. He currently serves as Deputy Node Leader for the DSTI-NRF Centre of Excellence in Mathematical and Statistical Sciences (CoE-MaSS) and is the 2025 Track Chair for Computational and Data-Driven Modelling at the RAPDASA–RobMech–PRASA–AMI Conference.

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