Africa-UK Partnership for the Computer-aided Development of Sustainable Catalysts

David Santos-Carballal[a,b,*] [§], Cornelia G.C.E. van Sittert[c] and Nora H. de Leeuw[a,b]

[a]*School of Chemistry, University of Leeds, Leeds LS2 9JT, UK.*
[b]*School of Chemistry, Cardiff University, Park Place, Cardiff CF10 3AT, UK.*
[c]*Laboratory for Applied Molecular Modelling, North-West University, Private Bag X6001, Potchefstroom, 2520, South Africa.*

Collaboration is the cornerstone of modern science, driving the development of new knowledge, concepts, methodologies, and thought processes. The complementary expertise existing in South Africa, Ghana, Botswana, Namibia, and the United Kingdom has allowed the advancement in the field of sustainable catalysis showcased in the thematic issue of the *South African Journal of Chemistry*, to which this foreword is an introduction.

Historically, the design, testing and characterization of the catalyst structure and analysis of reactants, intermediates, and products, has been at the centre of catalysis science. However, the advent of computer modelling has underpinned the predictive simulation of the geometries and properties of catalysts and their interaction with reactants, intermediates, and products. The inspection and assessment of simulated catalytic pathways and the effect of a range of environmental conditions have become an almost routine task in modern catalysis research, thereby supporting and complementing experiments. The modelling of various reaction mechanisms and the calculation of their kinetic and thermodynamic energy profiles has led to a new and realistic description of catalytic processes.

The rapid progress of the computer-aided development of sustainable catalysts has been facilitated by innovative and accurate theoretical concepts and their implementation into a variety of software codes. The application of these computational tools to simulate complex systems and realistic problems have been driven by constantly expanding computational capacity. Most of the papers in this theme issue have used the South Africa National Centre for High Performance Computing (CHPC), the Cardiff University HPC systems, the pan-Wales network of computer clusters HPC Wales or its successor Supercomputing Wales (SCW), hosted by Cardiff University.

The articles in this theme issue exemplify many of the major challenges in the contemporary computer-aided development of catalysts and materials for sustainable energy. The topical simulation of the lithium intercalation voltage in spinel-structured materials is explored in the paper by Malatji *et al*.[1] In contrast, key issues in the development of computational models to describe cobalt and its oxide phases are addressed in the article of Cadi-Essadek *et al*.[2] The paper of Phaahla *et al*.[3] examines the phase transition in titanium nanoclusters using dynamic simulation methods, and the challenges in extrapolating binding energies to alkaline earth metal oxides are investigated by Escher *et al*.[4] In the contribution of Botchwaya *et al*.,[5] density functional theory calculations are used to model the surface and catalytic properties of zeolites. On the other hand, Meerholz *et al*.[6] deployed atomistic simulations based on interatomic potentials to provide new insight into the thermodynamics and structure of the atomic distribution in metal alloy surfaces. Nyeptesi *et al*.[7] have exploited *in situ* monitoring techniques to study the carbonate-catalyzed transesterification of sunflower oil for biodiesel production, whereas the hydrogenation of sorbic acid using Pd- and Ni-based complexes as catalysts is illustrated in the work of Olaoyea *et al*.[8] Finally, the article of Ungerer *et al*.[9] demonstrates the key importance of the competitive adsorption of water and sulfur oxide on platinum surfaces, while Peck *et al*.[10] examined the significance of the adsorption of hydrogen and oxygen on the surfaces of transition metals with varying magnetic ordering.

The science reported in this volume celebrates the success of two collaborative research consortia between scientists in the UK and several African countries. Both the Newton PhD exchange programme 'Computational Catalysis: a sustainable UK-South Africa partnership in high performance computing', funded jointly by the SA National Research Foundation and the UK Economic and Social Research Council (ESRC: grant number ES/N013867/1), and the 'New materials for a sustainable energy future' programme, funded by the UK Department for International Development (DFID) under the Royal Society Africa Capacity Building Initiative, have enabled the collaborative work presented in this special issue. One of the highlights of these international research programmes was the conference attended by the combined consortia on the Potchefstroom Campus of North-West University in April 2019, where the researchers had the opportunity to present the work published here and discuss future collaborations.

Finally, we are grateful to the *South African Journal of Chemistry* for their support of this theme issue. We hope that it illustrates the range and impact of the Africa-UK partnership for the computer-aided development of sustainable catalysts.

[§]ORCID iDs
D. Santos-Carballal: orcid.org/0000-0002-3199-9588
C.G.C.E. van Sittert: orcid.org/0000-0001-5786-5409
N.H. de Leeuw: orcid.org/0000-0002-8271-0545

References

1 K.T. Malatji, D. Santos-Carballal, U. Terranova, P.E. Ngoepe and N.H. de Leeuw, Controlling the lithium intercalation voltage in the $Li(Mn_{1-x}Ni_x)_2O_4$ spinel *via* tuning of the Ni concentration: a Density Functional Theory study, *S. Afr. J. Chem.*, 2021, **74** (Special Edition), 3–7.

2 A. Cadi-Essadek, A. Roldan, D. Santos-Carballal, P.E. Ngoepe, M. Claeys and N.H. de Leeuw, DFT+U Study of the electronic, magnetic, and mechanical properties of Co, CoO, and Co_3O_4, *S. Afr. J. Chem.*, 2021, **74** (Special Edition), 8–16.

3 T.M. Phaahla, A.A. Sokol, C. R. A. Catlow, S.M. Woodley, P.E. Ngoepe and H.R. Chauke, The thermal agitated phase transitions on the Ti_{32} nanocluster: a molecular dynamics simulation study, *S. Afr. J. Chem.*, 2021, **74** (Special Edition), 17–22.

4 S.G.E.T. Escher, H.D. Duncan, A.A. Sokol and S.M. Woodley, Approaching bulk from the nanoscale: extrapolation of binding energy from rock salt cuts of alkaline earth metal oxides, *S. Afr. J. Chem.*, 2021, **74** (Special Edition), 23–29.

* To whom correspondence should be addressed.
E-mail: d.santos-carballal@leeds.ac.uk

ISSN 0379-4350 Online / ©2021 South African Chemical Institute / http://saci.co.za/journal
DOI: https://doi.org/10.17159/0379-4350/2021/v74a1

5 C.H. Botchway, R. Tia, E. Adei, N.Y. Dzade and N.H. de Leeuw, H-FER-catalyzed conversion of methanol to ethanol and dimethyl ether: a first-principles DFT study, *S. Afr. J. Chem.*, 2021, **74** (Special Edition), 30–35.

6 K. Meerholz, D. Santos-Carballal, U. Terranova, A. Falch, C.G.C.E. van Sittert and N.H. de Leeuw, Thermodynamics of the atomic distribution in Pt_3Pd_2 and Pt_2Pd_3 and their corresponding (111) surfaces, *S. Afr. J. Chem.*, 2021, **74** (Special Edition), 36–41.

7 M. Nyepetsia, F. Mbaiwa, O.A. Oyetunji, N.Y. Dzade and N.H. de Leeuw, The carbonate-catalyzed transesterification of sunflower oil for biodiesel production: *in situ* monitoring and Density Functional Theory calculations, *S. Afr. J. Chem.*, 2021, **74** (Special Edition), 42–49.

8 O.E. Olaoye, O. Oyetunji, B.C.E. Makhubela, A. Muyaneza, G. Kumar and J. Darkwa, Catalytic hydrogenation of sorbic acid using pyrazolyl palladium(II) and nickel(II) complexes as precatalysts, *S. Afr. J. Chem.*, 2021, **74** (Special Edition), 50–56.

9 M.J. Ungerer, D. Santos-Carballal, C.G.C.E. van Sittert and N.H. de Leeuw, Competitive adsorption of H_2O and SO_2 on catalytic platinum surfaces: a Density Functional Theory study, *S. Afr. J. Chem.*, 2021, **74** (Special Edition), 57–68.

10 M.A. Peck, D. Santos-Carballal, N.H. de Leeuw and M. Claeys, Density Functional Theory study of the adsorption of oxygen and hydrogen on 3d transition metal surfaces with varying magnetic ordering, *S. Afr. J. Chem.*, 2021, **74** (Special Edition), 69–72.