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SUMMARY

I am a physical in the fields of computational material science and catalysis. My area of expertise spans the fields of quantum chemical modelling as well as experimental research and synthesis. During my postdoctoral studies I have investigated the integration of boron nitride nanotubes (BNNTs) into metals to form metal matrix composite (MMC) materials in an effort to test the feasibility and use of these materials for novel space and aircraft design in collaboration with NASA. The study resulted in winning an IRAD phase I project with NASA Langley Research Center in FY2016. In addition I examined possible CO_2 conversion pathways to hydrocarbons on minority phases of TiO_2 anatase. During my PhD I conducted extensive computational and experimental work investigating the adsorption and reaction behaviour of small molecules on metal oxide surfaces, and synthesised novel metal clusters during my Masters studies. My research was often conducted through collaboration visits for example Bochum Germany (Prof. Wöll), Denton, TX (Prof. Bagus), NASA Langley Research Center (LaRC), VA (Dr Park and Dr Yamakov) and Aberdeen, UK (Prof. Idriss).

EXPERTISE

- Employing quantum chemical calculations to aid experimental studies and to obtain insight on an atomic level that help to clarify and explain observed phenomenon
- Computer-based modelling of conversion and adsorption processes on metal oxides and the interaction of nano fibres with metals to form MMCs
- Applying experimental techniques (e.g. XPS, XRD, FTIR or RAIRS) to characterise the surface of metal and metal oxides and to validate computational results
- Supervision of postgraduate students in the field of computational chemistry
- Teaching of 1st through 3rd year science and engineering students in the field of chemistry during laboratory sessions and workshops

RESEARCH SKILLS

Computer and Modelling Skills

- Density Functional Theory (DFT) based simulations; packages - VASP (Vienna Ab Initio Simulation Package) and CASTEP (Cambridge Total Energy Package)
- Structure optimisation tools-SIRIUS and CHIMERA
- Cluster modelling packages - Alchemy
- Extensive experience utilising various high performing computing infrastructures
- Broad knowledge of Unix-and Windows-based operating systems
- Unix shell scripting

Experimental Techniques and Instrumentation Knowledge

- Surface analysis methods - FTIR and RAIRS
- Techniques determining the composition of metals and metal oxides – TEM, XPS and XRD
- Experience with the assembly and operation of ultra high vacuum systems

EDUCATION

PHD Chemistry, University of Auckland, New Zealand, January 2012
"Carbon Monoxide Adsorption onto the Metal Oxide of α-Al_2O_3 and Titania"

MSC Chemistry, University of Dresden, Germany, November 2006
"Synthesis, Characterisation and Crystal Structure Determination of $Ir_4CoSn_{18}O_{19}$ and $Ir_{10}CoSn_{45}O_{45}$"

PROFESSIONAL EXPERIENCE

07/2017 – Current ***Visiting Assistant Research Scientist, National Institute of Standards and Technology (NIST), Gaithersburg, MD, USA***

Within NIST I'm part of a team investigating the catalytic growth of Boron Nitride Nanotubes (BNNTs) and Carbon Nanotubes (CNTs) and their interaction with different metals by means of quantum chemical calculations. We collaborate closely with scientists from the NASA LaRC (NASA Langley Research Center) as well as from the University of Queensland.

05/2016 – 07/2017 ***Independent Research in collaboration with NASA LaRC and the University of Queensland***

I continued my research on boron nitride nanotube (BNNT) reinforced metal matrix composites focusing especially on Ti and Cu based MMCs, publishing several peer reviewed papers jointly with the NASA Langley Research Center and assisting with the presentation of our project at international research conferences. In addition I continue to investigate 2D materials for battery use employing different probe molecules to investigate the binding behaviour of strained surfaces.

05/2013 – 05/2016 ***Postdoctoral Research Fellow, Australian Institute for Bioengineering and Nanotechnology (AIBN), University of Queensland, Brisbane, Australia***

My research conducted at AIBN focused on the integration of BNNT fibres into a metal matrix to produce improved reinforced MMCs by means of DFT (VASP and CASTEP based). To gain a detailed understanding of the processes taking place at the interface the binding energies, charge distribution, density of states (DOS) and charge density difference plots for various BNNTs, metals and surface orientations were analysed. This research was conducted in close collaboration with NASA LaRC where the complimentary experiments were being conducted. While collaborating with NASA I visited the LaRC multiple times to present my research and stayed for an extended visit which was broadening my knowledge on

material performance testing methods, such as stress and strain and the synthesis procedure of the BNNT fibres. This knowledge enabled me to modify the theoretical models employed to more accurately simulate the systems and to make suggestions on the likelihood of certain metals to form the desired MMCs. My obtained computational results were also important in obtaining a NASA Internal Research and Development (IRAD) grant allowing for the continuation of this project. Just recently our collaboration with NASA was noted in aUQ press release (https://rcc.uq.edu.au/article/2016/05/flashlite-enables-uq-chemists%E2%80%99- work-nasa-identify-materials-spaceships-future).

I'm also part of a team investigating novel 2D materials which consist of different types of layered materials with potential use for future battery applications. In that regard I'm testing the strain that can be put on these materials before a significant reduction in binding/loading is noted.

Previously I was examining possible CO_2 conversion pathways on minority phases of TiO_2 anatase employing VASP. The obtained results of these projects were presented to NASA and NIA scientists, industry partner, at conferences, meetings and to funding agencies as well as published in peer reviewed journals.

My responsibilities at AIBN further included to identify funding opportunities and to apply for those ensuring all eligibility criteria are met, the presentation of the work conducted within our research group to industry such as SABIC and at networking events for students choosing a project for their Honours or PhD studies. In addition I was supervising undergraduate and postgraduate students in the field of quantum chemical calculations. I critically examined and analysed their obtained results and was aiding with the completion of their respective reports and theses.

01/2015 - 03/2015 ***Visiting Research Fellow, NASA-Langley Research Center (LaRC), Hampton, VA, U.S.***

During the collaborative research visit at the NASA LaRC facility I was consulting with experimental and theoretical scientists regarding the BNNT fibre MMCs investigation. I was able to examine the synthesis process, the final product and possible ways to alter the production process of BNNTs to improve their bonding with the metal matrix. Based on these findings, the discussions with the research staff and my computational results, new pathways and procedures for the experimental and quantum chemical approaches were discussed. While being at the LaRC facilities I presented my obtained results, often at short notice, to the BNNT group and associates. Currently the obtained theoretical and experimental results are being prepared for several joint publications.

02/2012 – 11/2015 ***Lead Demonstrator and ITAS tutor, School of Chemistry, University of Queensland, Brisbane, Australia***

I have been supervising the evening classes in the teaching laboratories in the School of Chemistry where I have managed and lead first year chemistry laboratory practical sessions, trained and mentored new laboratory tutors, and maintained high levels of safety compliance for staff, students and visitors. My responsibilities further included on site trouble shooting, altering procedures when necessary and a timely completion of the laboratory sessions.
In addition I was teaching in workshops and seminars of up to 200 participants for 1st through to 3rd year students. My teaching responsibilities further included the assessment of ITAS indigenous student's level of knowledge which included the identification of the students most effective way to study and to be taught. Furthermore I prepared and implemented teaching plans to achieve a specific objective according to their level of understanding and conducted a performance review of each student at the end of each semester. My efforts were recognized by obtaining a teaching award based on student and staff evaluations. In addition it made me the preferred choice for chemistry of the ITAS management team.

03/2011– 08/2011 ***Research Fellow, Eskitis Institute for Drug Discovery, Griffith University, Brisbane, Australia***

At the Eskitis institute I have been responsible for the analysis of a chemical library containing over 4000 small molecules. My duties involved the examination of each compound with respect to its structure and chemical integrity. I independently optimised and corrected all erroneous or misrepresented molecules with the SIRIUS and CHIMERA optimisation packages.

TOP THREE CAREER ACHIEVEMENTS

Boron nitride nanotubes as metal reinforcement The first publication listed was conducted in close collaboration with the NASA LaRC and demonstrates that boron nitride nanotubes can potentially be integrated into an Al, Ti and Cu metal matrix. This played a significant role in securing a NASA IRAD grant to further investigate the composite on an experimental level.

Direct monitoring of CO oxidation The fifth publication listed below (cited nearly 40 times) shows that the catalytic oxidation of CO to CO_2 on a TiO_2(110) well defined single crystal is a direct, one step process. This study was the first of its kind employing a specially designed RAIRS apparatus that allowed resolution high enough to directly monitor the adsorption and conversion process.

Lowest energy barrier for CO_2 at the (105) TiO_2 face of anatase The third publication listed reveals the mechanism for the electrochemical conversion of CO_2 into different hydrocarbon compounds with the TiO_2(105) anatase surface showing significantly lower energy barriers compared to all other major and minor surfaces investigated.

COMPETETIVE RESEARCH GRANTS

D. J. Bernhardt, **C. Rohmann**. Composite reinforcement using boron nitride nanotubes, Asian Office of Aerospace Research and Development, Research Grant 2014
Grant number: AOARD 144017
Funding $50k (June 2014, 1 year)

D. J. Bernhardt, **C. Rohmann**. Composite reinforcement using boron nitride nanotubes, Asian Office of Aerospace Research and Development, Research Grant 2013
Grant number: AOARD134071
Funding $50k (June 2013, 1 year)

LIST OF PUBLICATIONS AND PRESENTATIONS

PUBLICATIONS

1. **C. Rohmann**, Q. Sun and D. J. Searles. The Interaction of Al, Ti and Cu Atoms with Boron Nitride Nanotubes (BNNTs): A Computational Investigation. *J. Phys. Chem. C,* **2016**, *120, 3509-3518.*
2. **C. Rohmann**, J. B. Metson, H. Idriss. A DFT Study on Carbon Monoxide Adsorption onto hydroxylated α-Al_2O_3(0001) surfaces. *Phys. Chem. Chem. Phys.*, **2014,** *16* 14287–14297
3. **C. Rohmann**, C. H. Sun and D. J. Searles. CO_2 Activation and Conversion on Majority and Minority Faces of TiO_2 Anatase. *Abstract of Paper of the American Chemical Societ*, Dallas, TX, United States **March 2014**
4. **C. Rohmann**, J. B. Metson, H. Idriss. DFT study of carbon monoxide adsorption on α-Al_2O_3(0001). *Surface Science***, 2011**, *605*, 1694–1703
5. **C. Rohmann**, Y. Wang, M. Muhler, J. Metson, H. Idriss, C. Wöll. Direct monitoring of photo-induced reactions on well-defined metal oxide surfaces using vibrational spectroscopy. *Chemical Physics Letters*, **2008,** *460*,10–12
6. T. Söhnel, L. Kienle, **C. Rohmann**, M. Ruck and F E. Wagner. Tin Clusters under the Electron Microscope? The real structure of $Ir_4CoSn_{19}O_{18}$ and $Ir_{10}CoSn_{45}O_{45}$. *Proceedings of the 32th Annual Condensed Matter and Materials Meeting,* **2008** *27*:1-4
7. T. Söhnel, **C.Rohmann**, M. Ruck, L. Kienle., F. E. Wagner. Crystal Structure and Characterization of $Ir_4MSn_{18}O_{19}$ and $Ir_{10}CoSn_{45}O_{45}$. *Proceedings of the NZIC,* **2006,** *2*, 91-93

ORAL AND POSTER PRESENTATIONS

1. **C. Rohmann**, Q. Sun and D. J. Searles. Composite Reinforcements using Boron Nitride Nanotubes. *Molecular Modelling*, **July 2014**, Lammington National Park, Queensland, Australia (Poster Presentation)
2. **C. Rohmann**, C. H. Sun and D. J. Searles. CO_2 Activation and Conversion on Majority and Minority Faces of TiO_2 Anatase. *ACS Conference*, **March 2014**, Dallas, TX, U.S. (Oral Presentation)
3. **C. Rohmann** and H. Idriss .The Adsorption of CO onto the dry surface of α-Al_2O_3(0001*). Auckland Research Showcase* The University of Auckland, Auckland, New Zealand, **June 2009** (Poster Presentation)
4. **C. Rohmann** and H. Idriss. The Adsorption of CO onto the dry surface of α-Al_2O_3(0001). *Joint Symposium of the Collaborative Research Centres 546 (Berlin) and 558 (Bochum),* Erkner near Berlin, **October 2007** (Poster Presentation)