



Contribution ID: 165

Type: **Invited Talk**

## Computational Catalysis @ NWU

*Wednesday, 4 December 2019 13:30 (20 minutes)*

At the North-West University (NWU) interest in incorporating computational chemistry in training and research started in the late 1990. Although there was not much support for this interest in computational chemistry, the need for understanding the chemistry in especially catalysis was identified.

Starting with old discarded computers and the cheapest possible software, the first attempts were made in calculating structures of transition metal complexes used in catalysis research at NWU. Due to the limitation of the resources, only gas phase reactions in homogeneous catalysis could be investigated. As the value of the computational investigations became evident, more resources were acquired.

It was however only in 2002 that support from the Research Focus Area (previously called Separation Technology) at NWU was obtained. Formal training of one staff member and the establishment of a dedicated Laboratory for Applied Molecular Modelling was funded. After careful evaluation of the needs in the research and the abilities of the researchers, it was decided to invest in Accelrys Materials Studio (for research) and Spartan (for training) software. At the same time 10 workstations and a 12 CPU cluster were acquired.

Although this was a major step forward, catalysis research was still limited to gas phase reactions in homogeneous catalysis investigations, with transition state calculations being a challenge. At this stage the CHPC was established. After a short phase of development and streamlining operations and software at CHPC, access to these resources were obtained by NWU researchers.

With the access to CHPC resources, limitations to the type of investigations gradually disappeared. The homogeneous catalysis investigations could be expanded to real system investigation, including solvents. Models could be expanded from explanations of observations to prediction for activity. Heterogeneous catalysis could also be included in research.

Now, computational catalysis research at NWU was ready to investigate real problems and try to find solutions. One such real problem being investigated at NWU is the development of new/alternative catalysts to apply in the generation of alternative and renewable energy.

### Supported Student

**Primary author:** Prof. VAN SITTERT, Cornie (North-West University)

**Presenter:** Prof. VAN SITTERT, Cornie (North-West University)

**Session Classification:** HPC Applications

**Track Classification:** Computational Chemistry