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Computational Chemistry within the Laboratory of Applied Molecular Modelling at NWU

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In 2002 with support from the Research Focus Area (Separation Technology) at North-West University (NWU), the Laboratory for Applied Molecular Modelling (LAMM) was established. After the evaluation of the researchers' abilities and the research needs, an investment was made in Accelrys Materials Studio software. Additionally, ten workstations and a 12 CPU cluster were acquired. The focus of the research done at that time in the LAMM was homogeneous catalysis, which was limited to reactions in the gas phase. Transition state calculations, as well as reaction in solutions, were a challenge.

Around the same time, the CHPC was established. However, only on 23 January 2016, the application to register a program at the CHPC was approved. The title of this program is: "Computational Chemistry within the Laboratory of Applied Molecular Modelling at NWU".

Within this program, the LAMM supports and facilitates the use of computational chemistry in research at NWU. The projects that ran between January 2016 and March 2018 was: 1. Solvent extraction of Ta, Nb, Hf and Zr from various minerals; 2. Polymer Blends - a collaboration with UFS and Qatar University. 3. Identification of mechanisms in biochemistry; 4. Homogeneous and Heterogeneous catalysis; 5. Collaboration with a group in China on polyphosphazenes; and 6. Interfaces in crystals with mechanical engineering at NWU. In this period (26 months), the program used 213896 CPU hours per month. Since then, some projects ran to completion, some were added, some were completed, and some expanded. The CPU hours have increased to 790636 CPU hours per month.

The project that expanded the most is "Homogeneous and Heterogeneous catalysis", specifically heterogeneous catalysis. The focus in heterogeneous catalysis is on developing new/alternative catalysts to apply in the generation of alternative renewable energy and pollution control.

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