Contribution ID: **258** Type: **Talk**

HPC insights into chemistry mysteries

Tuesday, 4 December 2018 14:30 (20 minutes)

This contribution is aimed to illustrate how chemical computational results, obtained by density functional theory calculations on high performance computers, provides insight into many observed chemical phenomena, mysteries or questions, such as the following:
The structure of water clusters in bulk water is considered one of the unsolved problems in chemistry. How does the structure of water clusters look like at nanoscopic scale? How do the connecting hydrogen bonds render water ideally suited to life processes, being easily formed but not too difficult to break? A photochromic mercury compound has an orange colour in solution, but turns blue when sunlight shines on it. Why? How do these orange and blue forms differ in structure? Why is conductivity much higher for a certain iridium complex, than for the related rhodium complex with the same ligand? Why is the transient reaction intermediate within a multi-step red blood cell reaction not experimentally observable?
These and many other puzzling chemical problems, can be addressed very efficiently without experimental error, by computational chemistry conducted on high performance computers, thereby bypassing tedious or expensive laboratory techniques.

References:
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Presenter Biography

Jeanet Conradie obtained her Ph.D. in Chemistry in 2000, from the University of the Free State, South Africa, where she now is a Professor in Physical Chemistry. Her current research interests involve the synthesis, structure, electrochemistry, kinetics and density functional theory (DFT) calculations of novel transition metal complexes and their intermediates. She applies computational methods to predict or shed light on experimental observation.

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Session Classification: HPC Applications

Track Classification: Computational Chemistry