Computational Chemistry at the University of Mauritius: Past, Present & Future

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Computational chemistry involves the use of theoretical methods and computers to solve chemical problems. It has progressed with the explosive increase of computational power and availability of user-friendly software.

It will be almost twelve years that computational chemistry has been introduced at the University of Mauritius. This presentation gives an overview of the development of computational chemistry at the University of Mauritius both at academic and research levels. Before the year 2000, this component of chemistry was not known at this University but now a computational chemistry module is running successfully at undergraduate and postgraduate levels.

A computational chemistry group has been established with research students and renowned researchers across the globe. Our computational chemistry group focuses on research in four distinct areas namely: (1) Isolated novel molecules; (2) Global warming species; (3) Reaction mechanism and (4) Drug development.

Computational chemistry provides the possibility to predict the structural, kinetics and thermodynamic parameters of chemical systems.

Studies on isolated novel molecules have been reported with respect to their structural parameters, ionisation energy, dissociation energy and electron affinity. Global warming gaseous species have been studied to determine the global warming potential. Mechanisms of reactions have been probed and the most feasible pathway proposed based on calculation of thermodynamic functions, rate constant and reactivity indices. Novel compounds have also been studied in terms of commonly referred indices to evaluate their suitability as potential drug candidates.

Therefore, computational chemistry offers a wide choice of menu for chemical education and research. There are challenges ahead but our inspiration is derived from "*Try and Try Until you Succeed*….".