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The use of Gaussian 09 to identify trends in the optical properties and electronic structures of porphyrin and BODIPY dyes

The use of the Gaussian 09 software package on the Lengau cluster to carry out DFT and TD-DFT calculations to identify structure-property relationships in the properties of porphyrin [1] and BODIPY [2] dyes will be described. An analysis of the DFT and TD-DFT calculations for these dyes can provide an insight into their electronic structures and hence guide the rational design of novel dyes for applications such as photodynamic therapy [3,4] and optical limiting [5-7].

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Presenter Biography

Dr. John Mack graduated from Aberdeen University in Scotland in 1988 and carried out his PhD studies at the University of Western Ontario in Canada under the supervision of Prof. Martin Stillman. The use of Fortran software to collect and analyze the optical and redox data of phthalocyanine dyes formed an important part of this research. Later, during postdoctoral research with Prof. Martin Stillman in Canada and as an assistant professor in the laboratory of Prof. Nagao Kobayashi at Tohoku University in Sendai, Japan, Dr. Mack studied how trends in the theoretical calculations of porphyrin and phthalocyanine dyes can be used to guide their rational synthesis. Since 2012, Dr. Mack has beeing working as a Senior Researcher at the Centre for Nanotechnology Innovation at Rhodes University and has been using this approach to identify porphyrin and BODIPY dyes that are suitable for nanotechnology applications.

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