



Contribution ID: 32

Type: **Talk**

Rational design of Sn(IV) porphyrins for photodynamic therapy: further progress and future perspectives

Thursday, 2 December 2021 14:30 (30 minutes)

Over the last year, considerable further progress has been made in using a rational design approach [1] guided by calculations with the Gaussian 09 software package on the Lengau cluster and an application of Michl's perimeter model [1,2] to prepare novel Sn(IV) complexes of porphyrin dyes and porphyrin analogues that are suitable for use as photosensitizer dyes in photodynamic therapy [3-8]. Axial ligation results in low levels of aggregation, while the Sn(IV) ion promotes intersystem crossing resulting in relatively high singlet oxygen quantum yields through a heavy atom effect. Relatively low IC₅₀ values have been obtained during *in vitro* studies against MCF-7 breast cancer cells [3-9]. Future directions on the use of the Gaussian 09 software package in the context of this research will be described.

References

- [1] J. Mack, *Chem. Rev.* **2017**, *117*, 3444-3478.
- [2] J. Michl, *Tetrahedron* **1984**, *40*, 3845-3934.
- [3] B. Babu, J. Mack, T. Nyokong, *Dalton Trans.* **2020**, *49*, 9568-9573.
- [4] B. Babu, E. Prinsloo, J. Mack, T. Nyokong, *New J. Chem.*, **2020**, *44*, 11006-11012.
- [5] B. Babu, J. Mack, T. Nyokong, *Dalton Trans.* **2020**, *49*, 15180-15183.
- [6] B. Babu, J. Mack, T. Nyokong, *Dalton Trans.* **2021**, *50*, 2177-2182.
- [7] B. Babu, J. Mack, T. Nyokong, *New J. Chem.*, **2021**, *45*, 5654-5658.
- [8] R.C. Soy, B. Babu, J. Mack, T. Nyokong, *Dyes Pigments*, **2021**, *194*, 109631.
- [9] B. Babu, A. Sindelo, J. Mack, T. Nyokong, *Dyes Pigments*, **2021**, *185A*, 108886.

Student?

No

Supervisor name

Supervisor email

Primary author: Prof. MACK, John (Rhodes University)

Co-authors: Dr BABU, Balaji (Rhodes University); Ms SOY, Rodah (Rhodes University); Mr MAY, Aviwe (Rhodes University); Ms MOLUPE, Nthabeleng (Rhodes University); Ms CHIYUMBA, Choonzo (Rhodes University); Ms LEDWABA, Mahlatse (Rhodes University); Ms MAGWAZA, Temlandvo (Rhodes University); Prof.

TASSO, Thiago (Federal University of Minas Gerais); Prof. BAPTISTA, Mauricio (University of Sao Paulo); Prof. NYOKONG, Tebello (Rhodes University)

Presenter: Prof. MACK, John (Rhodes University)

Session Classification: HPC Applications

Track Classification: Computational Chemistry