RHODES UNIVERSITY, GRAHAMSTOWN, SOUTH AFRICA

STAFF INFORMATION

PROF JOHN MACK

Associate Professor - Research

CONTACT DETAILS:

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EDUCATION DETAILS:

Undergraduate:	1st Oct 1984 - 30th Jun 1988 Aberdeen University, Scotland B.Sc. in Chemistry (*First Class Honours*)
Postgraduate:	1st Sep 1988 - 30th Jun 1994 University of Western Ontario, Canada Ph.D. in Chemistry
Thesis:	MCD Spectroscopy of Phthalocyanine Anions (*Completed in June 1994 to fulfil requirements of Ph.D. degree*)

SCHOLARSHIPS AND AWARDS:

Undergraduate:	Coutts Prize for Chemistry in 1985-86 & 86-87. Forbes Prize for Physical Chemistry in 1987-88.
Postgraduate:	Ontario International Fee Waiver 1988-1994.
Research Funding:	Competitive Support for Unrated Researchers (CSUR) grant

National Research Foundation (NRF) from 2015-17
(Grant No: 93627)

China / South Africa Research Cooperation Programme with Prof. Zhen Shen (Nanjing University) for 2015-16
(Grant No: 95421)

WORK EXPERIENCE:

Work Experience

1st Jul 1994 - 31st Mar 1997	Postdoctoral Fellow	University of Western Ontario (*Prof. Martin J. Stillman*)
1st Apr 1997 - 31st Mar 1999	Research Associate	University of Western Ontario (*Prof. Emeritus James R. Bolton*)
1st Apr 1999 - 12th Oct 2004	Research Associate	University of Western Ontario (*Prof. Martin J. Stillman*)
13th Oct 2004 - 31st Jul 2006	Centre of Excellence Fellow	Tohoku University (*Prof. Nagao Kobayashi*)
1st Aug 2006 - 17th Sep 2007	Research Associate	University of Western Ontario (*Prof. Martin J. Stillman*)
18th Sep 2007 - 31st Mar 2010	Assistant Professor	Tohoku University (*Prof. Nagao Kobayashi*)
1st Apr 2010 - 31st Mar 2012	Research Associate	Tohoku University (*Prof. Nagao Kobayashi*)
1st Apr 2012 – 31 Dec 2019	Senior Researcher/ Nanotechnology Specialist	Rhodes University, Chemistry Dept, RU/DST Institute for Nanotechnology Innovation Direction: Prof T Nyokong
1st Jan 2020 – date	Associate Professor - Research	Rhodes University, Chemistry Dept, RU/DST Institute for Nanotechnology Innovation Direction: Prof T Nyokong

RESEARCH EXPERIENCE:

Photophysics

During my time at Rhodes University I have gained considerable experience in the maintenance and operation of Ekspla NT 342B and Quanta-Ray Nd/YAG lasers and a Lambda Physic FL 3002 dye laser to carry out triplet state lifetime and quantum yield measurements and to calculate singlet oxygen quantum yields using an ultra-sensitive germanium detector (Edinburgh Instruments, El-P) for phthalocyanines and porphyrins and their nanoparticle-conjugates. I have also supervised the use and maintenance of Picoquant Fluotime 200 and 300 fluorescence lifetime spectrometers and have carried out various fluorescence and phosphorescence measurements including both steady

	state emission spectra and the lifetimes of singlet and triplet excited states. Studying the effect of different types of modification to the structure of porphyrinoid ligands and other types of dye molecule such as boron dipyrromethenes (BODIPYs) and their analogues on the observed Φ_F and $\Phi_{\square}$ values is an obvious future research direction.
MCD spectroscopy	I have extensive experience in measuring and analyzing magnetic circular dichroism (MCD) spectra at both room and cryogenic temperatures. Although the MCD technique is somewhat specialized, it often provides key insights on the electronic structures of high symmetry heteroaromatic compounds, such as porphyrins and phthalocyanines, which are not readily available using other characterization methods. During my time at Tohoku University, my research largely focused on using Michl's perimeter model (a conceptual framework used to analyze the results of MO calculations of aromatic and heteroaroamatic □-systems) to identify key trends in the electronic structures of structurally related porphyrinoid compounds which shape the optical and redox properties. I have also studied the MCD spectroscopy of hemes in the context of the iron-regulated surface determinant proteins of the *Staphyloccocus aureus* hospital superbug to derive information about the spin state of the central ferrous or ferric ion and its coordination environment within the protein. The chemistry department at Rhodes University has purchased a Chirascan plus spectrodichrometer equipped with a 1 T (tesla) permanent magnet with a permanent magnet. I have recently assisted several postgraduate students at Rhodes University in the use of the MCD technique.
Theoretical calculations	I have carried out TD-DFT and INDO/s calculations on a wide range of porphyrinoids synthesized by over a dozen different research groups from around the world. Trends observed in the MCD spectra of structurally related porphyrinoids have been used to validate the theoretical descriptions of the electronic structures. One of my main research goals is to use molecular modelling and Michl's perimeter model to carry out the rational design and synthesis of novel porphyrinoids that are suitable for use in practical applications such as dye-sensitized solar cells and near-IR fluorescent dyes. Recent collaborative research on BODIPY and aza-BODIPY dyes with Prof. Zhen Shen of Nanjing University and Dr. Hua Lu of Hangzhou Normal University has provided an opportunity to apply insights derived from research on porphyrinoids to a wider range of dye molecules. During my time at Rhodes University, I have made extensive use of the sun cluster at the Centre for High Performance Computing in Cape Town and have instructed students how to carry out modelling calculations and analyze the results.
Electrochemistry	I have extensive experience in carrying out cyclic voltammetry and differential pulse voltammetry measurements. During my doctoral research in Prof. Martin Stillman's laboratory at the University of Western Ontario, I successfully designed cells which enabled CV and DPV measurements to be made under an inert atmosphere using a minimal amount of solution and supporting electrolyte. I also designed cells for use in the sample bore of a superconducting magnet to enable *in situ* spectroelectrochemical measurement of the MCD spectra of highly air-sensitive □-anion radical species. The redox properties of porphyrinoids

	are an ongoing area of interest, since they are directly related to the same trends in the electronic structure that are also studied by optical spectroscopy and theoretical calculations, and also play a key role in determining whether porphyrinoids are suitable for practical applications.
Photochemistry	During my doctoral research, I also gained considerable experience in using photochemistry to generate highly air-sensitive porphyrinoid □-anion radical species *in vacuo* for spectroscopic measurements. I subsequently studied the spectroscopy of air stable □-anion radical species of porphyrinoids with novel structures, which result in marked decreases in the first reduction potential. These species could be used in artificial photosynthesis and catalysis applications. Currently, it is only the □□cation radicals of porphyrinoids that tend to be used in this context, since most □-anion radicals are highly air-sensitive. A key future research goal would be to use Michl's perimeter model and the trends predicted in TD-DFT calculations to carry out the rational design and synthesis of the phthalocyanine analogues which are best suited to this type of research.
CD spectroscopy	I wrote a book with Prof. Nagao Kobayashi of Tohoku University on the theory of CD and MCD spectroscopy and the quantitative analysis of the spectral data derived from these techniques, which was published by the Royal Society of Chemistry in 2011. I have carried out a limited amount of research on the CD spectroscopy of aza-BODIPY dyes and other optically active polymers and complexes. Many researchers find the quantitative approaches to the analysis of CD spectral data quite challenging, so there is scope for collaborative research in this regard.
EPR spectroscopy	I have considerable experience in measuring and analyzing the EPR spectra of air sensitive paramagnetic porphyrinoid radical species at both room and cryogenic temperatures, including experiments at *ca.* 4 K in which liquid helium was used as the coolant. My experience with several different specialist spectroscopic techniques could be readily applied to a wide range of projects in inorganic and bioinorganic chemistry. Since moving to Rhodes University, I have supervised the use of a Bruker EMX plus instrument by students.
TOF-SIMS	An ION-TOF TOF-SIMS 5 instrument was recently installed at the RU/DST Centre for Nanotechnology Innovation at Rhodes University. I have been trained in its use and maintenance by a technician from the company and will be involved in measuring samples and supervising students in the use of the instrument.
XPS	I have received training on the use of a Kratos Analytical Axis Ultra DLD XPS instrument and will be involved in the data analysis of samples.
Software Development	I have had extensive experience in developing in house software to carry out highly specialized types of data analysis related to MCD spectroscopy such as the simultaneous spectral band deconvolution analysis of UV-visible absorption and MCD spectra and deriving values for excited state magnetic moments from $\mathbf{A_1/D_0}$ ratios. I also developed software to provide user interfaces, which enabled the remote control of Jasco and Cary spectrometers and a Princeton Applied Research potentiostat, prior

	to this type of software becoming commercially available. There is considerable scope for applying this experience in the present day based in the use of application macros.
Analytical Chemistry	In the late 1990s, I spent two years carrying out analytical chemistry research on the treatment of wastewaters using H_2O_2 and UV light. The research was largely funded by Calgon Carbon one of the leading companies in the field and involved close collaboration with an industrial R&D team. HPLC, GC, IC and colorimetric methods were used to monitor the progress of the wastewater treatments.

TEACHING EXPERIENCE:

Teaching Assistant	During my doctoral studies at the University of Western Ontario, I was involved on a twice weekly basis with laboratory courses for 2nd and 3rd year undergraduates. The primary focus in the 2nd year course was on the synthesis of inorganic compounds, while the 3rd year course focused on analytical chemistry with students provided hands on experience with IC, HPLC, GC and AAS equipment supplied by Varian. The experiments were geared towards the analysis of environmental samples and preparing students for careers in industry.
Postdoctoral Fellow	During my postdoctoral studies in Canada, I gained considerable experience in working closely with 4th year undergraduates during the course of research projects. The projects focused either on the synthesis and characterization of porphyrinoids and/or their paramagnetic anion and cation ??radical species or on the analysis of the treatment of environmental contaminants, such as methyl tertiary butyl ether, in waste waters using H_2O_2 and UV light.
Assistant Professor	During my time at Tohoku University, I prepared a 2nd year inorganic chemistry course for international exchange students using Shriver & Atkins as the textbook. I delivered ten 90 minute lectures and set the examinations for the course. I also participated in a laboratory course designed to teach the basics of the synthesis and characterization of inorganic compounds to Japanese 2nd year undergraduates. I actively participated in weekly group seminars in Prof. Nagao Kobayashi's laboratory in which 3rd and 4th year undergraduates and M.Sc. and Ph.D. students present their results. I have gained considerable insight into how significant progress can be achieved in porphyrinoid research by carefully designing narrowly focused research projects for undergraduates, which can be completed in a relatively short timeframe.
Senior Researcher	I currently teach a fourteen lecture second year course on spectroscopy and analytical chemistry, an eight lecture third year course on photochemistry, and ten lecture honours modules on spectroscopic techniques and porphyrinoid chemistry in the Chemistry Department at Rhodes University. The goal of the honours modules is to introduce students to the theoretical background that underpins much of the research carried out at the RU/DST Centre for Nanotechnology Innovation. One honours student and four MSc students are currently

working on my projects on the synthesis, properties and applications of phthalocyanine and BODIPY dyes. I recently obtained a Competitive Support for Unrated Researchers (CSUR) grant for *ca.* R 0.8 million and a China / South Africa Research Cooperation Programme grant for R 0.2 million from the National Research Foundation (NRF) of South Africa to fund this research until the end of 2017.

PUBLICATIONS:

Books [1]

1. N. Kobayashi, A. Muranaka and J. Mack, "Circular Dichroism and Magnetic Circular Dichroism Spectroscopy for Organic Chemists", Royal Society of Chemistry, London, **2011**. http://www.rsc.org/shop/books/2011/9781847558695.asp

Book Chapters [4]

1. J. Mack and M. J. Stillman, "Electronic Structure of Metal Phthalocyanine Complexes from the Analysis of the UV-Visible Absorption and Magnetic Circular Dichroism Spectra and Molecular Orbital Calculations", In "*The Porphyrin Handbook*", K. Kadish, K. Smith and R. Guilard, Eds., Academic Press, New York, **2002**, Vol. 16, Ch. 103, pp 43-116. http://www.sciencedirect.com/science/book/9780080923901
2. J. Mack and M. J. Stillman, "Magnetic Circular Dichroism (and Magnetic Optical Rotatory Dispersion)", In "*Application of Physical Methods to Inorganic and BioInorganic Chemistry*", R. A. Scott, C. M. Lukehart, Eds., John Wiley & Sons, New York, **2007**, 189-204. http://eu.wiley.com/WileyCDA/WileyTitle/productCd-0470032170.html
3. J. Mack and N. Kobayashi, "Recent Applications of MCD Spectroscopy to Porphyrinoids", In "*Multiporphyrin Arrays*", D. Kim, Ed., Pan Stanford Publishing, Ghaziabad, India, **2011**, 91-147. http://www.panstanford.com/books/9789814316606.html
4. J. Mack, N. Kobayashi, and Z. Shen, "The Effect of Structural Modifications on the Properties of Porphyrinoids", In "*Handbook of Porphyrin Science*", K. Kadish, K. Smith and R. Guilard, Eds., **2012**, World Scientific, Singapore, Vol. 23, Ch. 109, 281-371. http://www.worldscientific.com/series/porsci

Reviews (*published in peer-reviewed journals*)

1. J. Mack and M. J. Stillman, "Assignment of the Optical Spectra of Metal Phthalocyanines through Spectral Band Deconvolution Analysis and ZINDO Calculations" *Coordination Chemistry Reviews* **2001**, *219–221*, 993-1032. http://dx.doi.org/10.1016/S0010-8545(01)00394-0
2. J. Mack, M. J. Stillman and N. Kobayashi, "Application of MCD spectroscopy to porphyrinoids" *Coordination Chemistry Reviews* **2007**, 251, 429-453. http://dx.doi.org/10.1016/j.ccr.2006.05.011
3. J. Mack and N. Kobayashi, "Low Symmetry Phthalocyanines and their Analogues", *Chemical Reviews* **2011**, *111*, 281-321. http://dx.doi.org/10.1021/cr9003049
4. H. Lu, J. Mack, Y. Yang and Z. Shen, "Structural modification strategies for the rational design of Red/NIR region BODIPYs", *Chemical Society Reviews* **2014**, 43, 4778-4823. http://dx.doi.org/10.1039/c4cs00030g
5. J. Mack, J. Stone and T. Nyokong, "Trends in the TD-DFT Calculations of Porphyrin and Phthalocyanine Analogues", *Journal of Porphyrins and Phthalocyanines* **2014**, *18*, 630-641.

http://dx.doi.org/10.1142/S108842461450045X

6. L. Gai, H. Lu, Z. Li, J. Mack, T. Nyokong, Z. Shen and N. Kobayashi, “Fluorescent Chemosensors for Fluoride-Ion Based on Organosilicon Compounds”, *Coordination Chemistry Reviews* **2015**, *285*, 24-51. http://dx.doi.org/10.1016/j.ccr.2014.10.009

7. H. Lu, J. Mack, T. Nyokong, Z. Shen, and N. Kobayashi, "Optically Active BODIPYs", *Coordination Chemistry Reviews* **2016**, *318*, 1-15. http://dx.doi.org/10.1016/j.ccr.2016.03.015

Research Papers (*published in peer-reviewed journals*)

8. J. Mack, S. Kirkby, E. A. Ough and M. J. Stillman, “Ground-State and Optical Spectrum of Metallophthalocyanine Radical Anions from Low-Temperature Magnetic Circular Dichroism Spectroscopy”, *Inorganic Chemistry* **1992**, *31*, 1717-1719. http://dx.doi.org/10.1021/ic00035a037

9. S. Radzki, J. Mack and M. J. Stillman, “Spectroelectrochemical and Photochemical Studies of Octaethylporphyrin Complexes. Magnetic Circular Dichroism Spectroscopy Studies of the Oxidation of Ce(IV) Octaethylporphyrin Sandwich Complexes”, *New Journal of Chemistry* **1992**, *16*, 583-589.

10. J. Mack and M. J. Stillman, “Photochemical Formation of the Anion Radical of Zinc Phthalocyanine and Analysis of the Absorption and Magnetic Circular Dichroism. Assignment of the Optical Spectrum of [ZnPc(□3)]⁻”, *Journal of the American Chemical Society* **1994**, *116*, 1292-1304. http://dx.doi.org/10.1021/ja00083a015

11. J. Mack and M. J. Stillman, “Band Deconvolution Analysis of the Absorption and Magnetic Circular Dichroism Spectral Data of Zinc Phthalocyanine at Cryogenic Temperatures”, *Journal of Physical Chemistry* **1995**, *95*, 7935-7945. http://dx.doi.org/10.1021/j100020a015

12. J. Mack and M. J. Stillman, “Assignment of the Optical Spectra of Metal Phthalocyanine Anions”, *Inorganic Chemistry* **1997**, *36*, 413-425. http://dx.doi.org/10.1021/ic960737i

13. J. Mack, N. Kobayashi, C. C. Leznoff and M. J. Stillman, “Absorption and Magnetic Circular Dichroism Spectra, and Molecaular Orbital Calculations of Tetrabenzotriazaporphyrins and Tetranapthotriazaprophyrins”, *Inorganic Chemistry* **1997**, *36*, 5624-5634. http://dx.doi.org/10.1021/ic961389n

14. J. Mack and J. R. Bolton, “Photochemistry of nitrite and nitrate in aqueous solution: a review”, *Journal of Photochemistry and Photobiology A* **1999**, *128*, 1-13. http://dx.doi.org/10.1016/S1010-6030(99)00155-0

15. M. I. Stefan, J. Mack and J. R. Bolton, “Degradation Pathways during the Treatment of Methyl *tert*-Butyl Ether by the UV/H_2O_2 Process”, *Environmental Science & Technology* **2000**, *34*, 650-658. http://dx.doi.org/10.1021/es9905748

16. J. Mack and M. J. Stillman, “Transition Assignments in the Ultraviolet-Visible Absorption and Magnetic Circular Dichroism Spectra of Phthalocyanines”, *Inorganic Chemistry* **2001**, *40*, 812-814. http://dx.doi.org/10.1021/ic0009829

17. J. Mack and M. J. Stillman, “Assignment of the Optical Spectrum of Metal Porphyrin and Phthalocyanine Radical Anions”, *Journal of Porphyrins and Phthalocyanines* **2001**, *5*, 67-76. http://dx.doi.org/10.1002/1099-1409(200101)5:1<67::AID-JPP300>3.0.CO;2-3

18. M. J. Stillman, J. Mack and N. Kobayashi, “Theoretical Aspects of the Spectroscopy of Phthalocyanines and Porphyrins”, *Journal of Porphyrins and Phthalocyanines* **2002**, *6*, 296-300. http://dx.doi.org/10.1142/S108842460200035X

19. N. Kobayashi, J. Mack, K. Ishii and M. J. Stillman, “Electronic Structure of Reduced Symmetry Peripheral Fused-Ring-Substituted Phthalocyanines”, *Inorganic Chemistry* **2002**, *41*, 5350-5363. http://dx.doi.org/10.1021/ic011152d

20. S. P. Keizer, J. Mack, B. Bench, S. Gorun and M. J. Stillman, "Electronic Structure and Spectroscopy of Electron Deficient Zinc Phthalocyanines", *Journal of the American Chemical Society* **2003**, *125*, 7067-7085. http://dx.doi.org/10.1021/ja0299710

21. J. Mack, C. L. Vermeiren, D. E. Heinrichs and M. J. Stillman, "In vivo heme scavenging by *Staphylococcus aureus* Isd C and Isd E proteins", *Biochemical and Biophysical Research Communications* **2004**, *320*, 781-787. http://dx.doi.org/10.1016/j.bbrc.2004.06.025

22. J. Mack, Y. Asano, N. Kobayashi and M. J. Stillman, "Application of MCD Spectroscopy and TD-DFT to a Highly Non-Planar Porphyrinoid Ring System. New Insights on Red Shifted Porphyrinoid Spectral Bands", *Journal of the American Chemical Society* **2005**, *127*, 17697-17711. http://dx.doi.org/10.1021/ja0540728

23. C. L. Vermeiren, M. Pluym, J. Mack, D. E. Heinrichs and M. J. Stillman, "Characterization of the Heme Binding Properties of *Staphylococcus aureus* IsdA", *Biochemistry* **2006**, *45*, 12867-12875. http://dx.doi.org/10.1021/bi0607711

24. J. Mack, N. Kobayashi and M. J. Stillman, "Magnetic Circular Dichroism spectroscopy and TD-DFT calculations of metal phthalocyanine anion and cation radical species", *Journal of Porphyrins and Phthalocyanines* **2006**, *10*, 1219-1237. http://dx.doi.org/10.1142/S1088424606000594

25. D. E. Heinrichs, J. Mack, M. Pluym, C. L. Vermeiren and M. J. Stillman, "Protoporphyrin IX and heme binding properties of *Staphylococcus aureus* Isd C", *Journal of Porphyrins and Phthalocyanines* **2007**, *11*, 165-171. http://dx.doi.org/10.1142/S1088424607000217

26. M. Pluym, C. L. Vermeiren, J. Mack, D. E. Heinrichs and M. J. Stillman, "Heme binding properties of *Staphylococcus aureus* Isd E", *Biochemistry* **2007**, *46*, 12777-12787. http://dx.doi.org/10.1021/bi7009585

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28. J. Mack, M. Bunya, Y. Shimizu, H. Uoyama, N. Komobuchi, T. Okujima, H. Uno, S. Ito, M. J. Stillman, N. Ono and N. Kobayashi, "Application of MCD Spectroscopy and TD-DFT to Non-Planar Core Modified Tetrabenzoporphyrins. Effect of Reduced Symmetry on Non-Planar Porphyrinoids", *Chemistry - A European Journal* **2008**, *14*, 5001-5020. http://dx.doi.org/10.1002/chem.200701611

29. J. Mack, M. Bunya, D. Lansky, D. P. Goldberg and N. Kobayashi, "The MCD Spectroscopy of Corrolazines and Triazatetrabenzocorroles", *Heterocycles* **2008**, *76*, 1369-1380. http://dx.doi.org/10.3987/COM-08-S(N)102

30. Z.-L. Xue, Z. Shen, J. Mack, D. Kuzuhara, H. Yamada, T. Okujima, N. Ono, X.-Z. You and N. Kobayashi, "A Facile One-Pot Synthesis of *meso*-Aryl-Substituted [14]Triphyrin(2.1.1)", *Journal of the American Chemical Society* **2008**, *130*, 16478-16479. http://dx.doi.org/10.1021/ja8068769

31. D. Kuzuhara, J. Mack, H. Yamada, T. Okujima, N. Ono and N. Kobayashi, "Synthesis, Structures, and Optical and Electrochemical Properties of Benzoporphycenes", *Chemistry - A European Journal* **2009**, *15*, 10060-10069. http://dx.doi.org/10.1002/chem.200900755

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35. Z. Xue, J. Mack, H. Lu, L. Zhang, X.-Z. You, D. Kuzuhara, M. Stillman, H. Yamada, S. Yamauchi, N. Kobayashi and Z. Shen, "The Synthesis and Properties of Free-Base [14]Triphyrin(2.1.1) Compounds and the Formation of Subporphyrinoid Metal Complexes", *Chemistry - A European Journal* **2011**, *17*, 4396-4407. http://dx.doi.org/10.1002/chem.201003100

36. H. Lu, S. Shimizu, J. Mack, X.-Z. You, Z. Shen and N. Kobayashi, "Synthesis and Spectroscopic Properties of Fused-Ring-Expanded Aza-BODIPYs", *Chemistry - An Asian Journal* **2011**, *6*, 1026-1037. http://dx.doi.org/10.1002/asia.201000641

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39. H. Lu, J Mack, J. Lei, X.-Z. You, N. Kobayashi and Z. Shen, "Facile Hg^{2+} Detection in Water using Fluorescent Self-Assembled Monolayers of a Rhodamine-Based Turn-on Chemodosimeter formed via a "Click" Reaction", *Journal of Materials Chemistry* **2011**, *21*, 10878-10882. http://dx.doi.org/10.1039/C1JM11319D

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9. J. Mack, M. Bunya, Y. Shimizu, H. Uno, M. J. Stillman, N. Ono and N. Kobayashi, "MCD spectroscopy and the effect of porphyrinoid ligand saddling: core modified tetrabenzoporphyrins", Fifth International Conference on Porphyrins and Phthalocyanines, Moscow, Russia, Jul 6th - 11th **2008**.
10. J. Mack, M. Bunya, Y. Shimizu, H. Uno, M. J. Stillman, N. Ono and N. Kobayashi, "The MCD spectroscopy of non-planar porphyrinoids" JSPS Global COE Symposium on Functional Materials and Analytical Approaches for Molecular Complex Chemistry, Sendai, Japan, Nov 5th - 6th **2008**.

11. J. Mack, “Modelling of spectra”, JSPS/NRF Joint Research Project Workshop on Understanding Spectra of Macrocyclic Compounds: linking experiments with theoretical calculations, Rhodes University, Grahamstown, South Africa, Feb 10th - 11th **2009**.
12. J. Mack, N. Kobayashi and M. J. Stillman, “MCD spectroscopy and TD-DFT calculations”, 2nd Georgian Bay International Conference on Bioinorganic Chemistry, Parry Sound, Canada, May 26th - 29th **2009**.
13. J. Mack, M. J. Stillman and N. Kobayashi, “MCD spectroscopy and TD-DFT calculations”, Sixth International Conference on Porphyrins and Phthalocyanines, Albuquerque, New Mexico, Jul 4th - 9th **2010**.
14. J. Mack, G. Kubheka, C. Mkhize, J. Stone, M. Wildervanck and T. Nyokong, “TD-DFT Calculations and MCD Spectroscopy: Analysis of the Structure-Property Relationships of Porphyrinoids”, Michinoku International Symposium on Porphyrins, Phthalocyanines and Functional □-Molecules, Zao, Japan, Oct 13th - 16th **2014**.
15. J. Mack, “TD-DFT Calculations and MCD Spectroscopy: Analysis of the Structure-Property Relationships of Porphyrinoids”, The 3rd National Symposium on Porphyrin Chemistry, Fuzhou, China, Dec 18th – 20th **2015**.
16. J. Mack, “Optical limiting and singlet oxygen generation properties of phosphorus triazatetrabenzcorroles”, Annual Research Symposium, Key Laboratory of Organosilicon Chemistry and Material Technology, Ministry of Education, Hangzhou Normal University, Hangzhou, China, Dec 22nd **2015**.

Invited/Keynote Speaker

1. J. Mack, “MCD spectroscopy and TD-DFT Calculations of Porphyrinoids”, Department of Chemistry, Rhodes University, Grahamstown, South Africa, Jun 3rd **2010**.
2. J. Mack, “Magnetic circular dichroism (MCD) spectroscopy and TD-DFT calculations of aromatic macrocycles”, State Key Laboratory of Coordination Chemistry, Nanjing National Laboratory of Microstructures, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing, Nov 26th **2012**.
3. J. Mack, “Magnetic circular dichroism (MCD) spectroscopy and TD-DFT calculations of aromatic macrocycles”, Key Laboratory of Organosilicon Chemistry and Material Technology Ministry of Education, Hangzhou Normal University, Hangzhou, China, Nov 27th **2012**.
4. J. Mack, “Analysis and rational design of near IR region dyes for biomedical and sensor applications”, School of Chemistry and Chemical Engineering, Jiangsu University, Zhenjiang, China, Dec 18th **2013**.
5. J. Mack, “Analysis and rational design of near IR region dyes for biomedical and sensor applications”, Key Laboratory of Organosilicon Chemistry and Material Technology Ministry of Education, Hangzhou Normal University, Hangzhou, China, Dec 20th **2013**.
6. J Mack, G Kubheka, J Harris, J Stone, Z Hlatshwayo, AK May, N Molupe, N Ndebele, BP Ngoy, T Nyokong
   Optical limiting properties of π–extended BODIPY and azaBODIPY dyes at 532nm
   10th International Conference On Porphyrins And Phthalocyanines (ICPP-10), Munich, Germany, 1-6 July **2018**
7. Prof John Mack Gugu Kubheka, Aviwe K. May, Nadine Dubazana, Nobuhle Ndebele,

Bokolombe P. Ngoy and Tebello Nyokong "Optical limiting properties of azaBODIPY and BODIPY dyes on the nanosecond timescale" 11th International Conference on Porphyrins & Phthalocyanines (ICPP-11) 28th June to 3rd July **2021** (Virtual Meeting)

8. Prof John Mack "Rational structural modification of porphyrins: NIR absorbing photosensitizer dyes for biomedical applications" 12th International Conference on Porphyrins & Phthalocyanines (ICPP-12), Madrid, Spain 10-15 July **2022**

9. Prof John Mack "Coordinated Porphyrinoids as Photosensitizers for Photodynamic Anticancer and Antimicrobial Chemotherapy" 5th Annual Conference of the Faculty of Science and Technology, University of Nairobi, Kenya 26 – 28 Oct **2022** (via zoom)

10. Prof John Mack, Roday Soy, Somila Dingiswayo, Kristen Burgess, Choonzo Chiyumba, Nthabeleng Molupe, Godfred Sebiawu, Mahlatse Ledwaba, Temlandvo Magwaza, Kaisano Tauyakhale, Tebello Nyokong
The photodynamic antimicrobial and anticancer activity properties of structurally analogous porphyrin, corrole, chlorin and N-confused porphyrin complexes
International Conference on Porphyrins and Phthalocyanines (ICPP-13)
Niagara Falls Convention Center Niagara Falls, Buffalo USA - 23-28 June **2024**

Oral Presentations

1. M. J. Stillman, J. Mack, S. Radzki and E. A. Ough, "Photochemical and Electrochemical Oxidation and Reduction of Metallophthalocyanines", The 7th Great Lakes Symposium in Photochemistry, University of Western Ontario, London, Ontario, May 3rd - 6th **1990**.
2. J. Mack and M. J. Stillman, "Spectroelectrochemistry of Magnesium Phthalocyanine Anions", The Eighth Annual Chemistry Graduate Student Symposium, State University of New York at Buffalo, May 23rd - 24th **1990**.
3. J. Mack and M. J. Stillman, "Photoreduction of Free Base and Metallophthalocyanines", The 25th Great Lakes ACS Regional Meeting, Marquette University, Milwaukee, Wisconsin, Jun 1st - 3rd **1992**.
4. M. J. Stillman, E. A. Ough and J. Mack, "Studies on Ring Oxidation and Ring Reduction in Phthalocyanines and Porphyrins by Magnetic Circular Dichroism Spectroscopy", The 38th Canadian Spectroscopy Conference, Trent University, Peterborough, Ontario, Aug 10th - 12th **1992**.
5. J. Mack and M. J. Stillman, "MCD Spectroscopy of Metal Phthalocyanine Anions", The 80th Canadian Chemical Conference and Exhibition, Windsor, Ontario, Jun 1st - 4th **1997**.
6. J. Mack and M. J. Stillman, "MCD Spectroscopy of Metal Phthalocyanine Anions", The 80th Canadian Chemical Conference and Exhibition, Windsor, Ontario, Jun 1st - 4th **1997**.
7. J. Mack and M. J. Stillman, "Photoreduction of Metal Phthalocyanine Complexes", Great Lakes Photochemistry Symposium, University of Western Ontario, London, Ontario, Jun 6th - 8th **1997**.
8. J. Mack, M. J. Stillman and N. Kobayashi, "The Application of Magnetic Circular Dichroism Spectroscopy to Sterically Hindered Non-Planar Porphyrin Ring Systems", The 87th Canadian Chemical Conference and Exhibition, London, Ontario, May 29th - Jun 1st **2004**.
9. J. Mack, M. J. Stillman and N. Kobayashi, "The Application of Magnetic Circular Dichroism Spectroscopy to Sterically Hindered Non-Planar Porphyrin Ring Systems", Third Midwest Metals Meeting, Ann Arbor, Michigan, Jun 4th - 6th **2004**.

10. J. Mack, N. Kobayashi and M. J. Stillman, "The application of magnetic circular dichroism spectroscopy to sterically hindered non-planar porphyrin ring systems", Third International Conference on Porphyrins and Phthalocyanines, New Orleans, Louisiana, Jul 11th - 16th **2004**.
11. J. Mack, "TD-DFT Calculations and MCD Spectroscopy: Ring-contracted, Fused-ring-expanded and Core Modified Porphyrinoids", Seventh International Conference on Porphyrins and Phthalocyanines, Jeju ICC, Korea, Jul 1st - 6th **2012**.
12. J. Mack, "The rational design of red/NIR region BODIPY dyes for sensor applications and PDT", 41st National Convention of the South African Chemical Institute, East London, South Africa, Dec 1st - 6th **2013**.
13. J. Mack, N. Kobayashi and Z. Shen, "TD-DFT Calculations and MCD Spectroscopy: identification of trends in the electronic structures and optical spectra of porphyrinoids", Eighth International Conference on Porphyrins and Phthalocyanines, Istanbul, Turkey, Jun 22nd - 27th **2014**.
14. J. Mack, G. Kubheka, C. Mkhize, J. Stone, M. Wildervanck and T. Nyokong, "TD-DFT Calculations and MCD Spectroscopy: Analysis of the Structure-Property Relationships of Porphyrinoids", The 17th SACI Inorganic Chemistry Conference, Grahamstown, South Africa, Jun 28th - Jul 2nd **2015**.
15. P. Majumdar, J. Zhao, J. Mack, Z. Shen and T. Nyokong, "Ir(III) Complexes Showing NIR Absorption/Emission For Application As Photodynamic Materials", The 17th SACI Inorganic Chemistry Conference, Grahamstown, South Africa, Jun 28th - Jul 2nd **2015**.
16. J. Mack, C. Mkhize, G. Kubheka, J. Britton, Z. Shen and T. Nyokong, "Optical limiting and singlet oxygen generation properties of phosphorus triazatetrabenzcorroles", Organometallic and Coordination Chemistry: Achievements and Challenges, Nizhny Novgorod, Russia, Sep 18th - 23rd **2015**.
17. M. Wildervanck, J. Mack and T. Nyokong, "Upconversion Nanoparticle-BODIPY conjugates for NIR activated singlet oxygen generation", 6th Annual DST/Mintek NIC Workshop, Grahamstown, South Africa, Oct 28th - 29th **2015**.
18. J. Mack, P. Majumdar, J. Harris, L. Gai, M. Shi, T. Nyokong, Z. Shen, "Rational design, synthesis and properties of non-benzo fused-ring-expanded phthalocyanines and aza-BODIPYs", Ninth International Conference on Porphyrins and Phthalocyanines, Nanjing, China, Jul 3rd - 8th **2016**.
19. J. Mack, P. Majumdar, J. Harris, L. Gai, M. Shi, T. Nyokong, Z. Shen, "Rational design, synthesis and properties of non-benzo fused-ring-expanded phthalocyanines and aza-BODIPYs", Twentieth Mendeleev Congress, Yekatarinburg, Russia, Sep 25th - 29th **2016**.
20. J. Mack, B. Babu, S. Dingiswayo, R. Soy, T. Tasso, M. Baptista, T. Nyokong
    Rational design of Sn(IV) porphyrins for photodynamic therapy: progress to date and future perspectives
    2020 Centre for High Performance Computing National Convention, Cape Town, Nov 30th – Dec 2nd 2020.
21. Mack, B. Babu, S. Dingiswayo, R. Soy, T. Tasso, M. Baptista, T. Nyokong
    Rational design of Sn(IV) porphyrins for photodynamic therapy: progress to date and future perspectives
    2020 Centre for High Performance Computing National Convention, Cape Town, Nov 30th – Dec 2nd 2020.

22. John Mack Gugu Kubheka, Aviwe K. May, Nadine Dubazana, Nobuhle Ndebele, Bokolombe P. Ngoy and Tebello Nyokong
Optical limiting properties of azaBODIPY and BODIPY dyes on the nanosecond timescale
11th International Conference on Porphyrins & Phthalocyanines (ICPP-11)
Hyatt Regency Buffalo/Hotel and Conference Center, Buffalo, New York, USA - 28th June to 3rd July 2021 (Virtual Meeting)

23. John Mack
Invited Speaker
Rational structural modification of porphyrins: NIR absorbing photosensitizer dyes for biomedical applications
12th International Conference on Porphyrins & Phthalocyanines (ICPP-12)
Madrid, Spain 10-15 July 2022

24. Prof. MACK, John; Dr BABU, Balaji; Dr MAY, Aviwe; Ms SOY, Rodah; Mr DINGISWAYO, Somila; Ms CHIYUMBA, Choonzo; Ms BURGESS, Kristen; Prof. NYOKONG, Tebello
Rational design of porphyrinoid dyes for photodynamic therapy: further progress and future perspectives
Centre for High Performance Computing 2022 National Conference
30 Nov 2 Dec, Gauteng, CSIR (via zoom meeting)

25. John Mack, Balaji Babu, Rodah Soy, Nthabeleng Molupe, Somila Dingiswayo and Tebello Nyokong
Group 13-15 Coordinated Porphyrinoids as Photosensitizers for Photodynamic Anticancer and Antimicrobial Chemotherapy
2nd BRICS Workshop on Biophotonics May 16 –18, **2023**, SARATOV, RUSSIA (via zoom)

26. C. Ji, J. Yang, S. Hu, J. Mack, Y. Zhang, H. Lu, L. Gai
Pyrrole hemithioindigo-derived organoboron complexes: synthesis, photophysical properties and its bioimaging applications", Dyes and Pigments 2023, 220, 111707
https://doi.org/10.1016/j.dyepig.2023.111707
Main Group Chemistry (IOS) via zoom

27. Prof John Mack
Metal corrole complexes for electrocatalytic hydrogen evolution reactions
7th International Symposium on Electrochemistry "Electrochemical Solutions for a Sustainable Future", Maharani Hotel in Durban, South Africa – 13 to 16 April 2025

Posters

28. J. Mack and M. J. Stillman, "Spectroelectrochemistry of Magnesium Phthalocyanine Anions", The 23rd Inorganic Discussion Weekend, University of Waterloo, Ontario, Nov 16th - 18th **1990**.
29. J. Mack and M. J. Stillman, "Spectroelectrochemistry of Magnesium Phthalocyanine Anions", The 74th Canadian Chemical Conference and Exhibition, Hamilton, Ontario, Jun 2nd - 6th **1991**.
30. M. J. Stillman, J. Mack and E. A. Ough, "Magnetic Circular Dichroism Spectroscopy of Phthalocyanine Anion Radicals and Cation Radicals", The 41st International Conference on Analytical Sciences and Spectroscopy, University of Windsor, Ontario, Aug 14th - 16th **1995**.
31. J. Mack and M. J. Stillman, "MCD Spectroscopy of Phthalocyanine Anions", The 42nd International Conference on Analytical Sciences and Spectroscopy, University of Western Ontario, Ontario, Aug 11th - 13th **1996**.

32. J. Mack and M. J. Stillman, "Molecular Orbital Calculations of the Optical spectra of Metal Phthalocyanine Complexes and Ring Oxidized and Reduced Species", The 80th Canadian Chemical Conference and Exhibition, Windsor, Ontario, Jun 1st - 4th **1997**.

33. J. R. Bolton, A. Safarzadeh-Amiri, S. R. Cater, B. W. Dussert, M. I. Stefan and J. Mack, "Mechanism and efficiency of the degradation of MTBE by the UV/H_2O_2 process", Southwest Focused Ground Water Conference, Anaheim, California, Jun 3rd - 4th **1998**.

34. J. Mack and J. R. Bolton, "The Impact of NO_2^- and NO_3^- on UV/H_2O_2 Processes", 1998 Pan American Workshop on Commercialization of Advanced Oxidation Technologies, London, Ontario, Jun 27th - 30th **1998**.

35. M. I. Stefan, J. R. Bolton, A. Safarzadeh-Amiri, J. Mack, S. R. Cater and B. W. Dussert, "Degradation Pathways during the Phototreatment of Methyl-*tert*-Butyl Ether by the UV/H_2O_2 Advanced Oxidation Process", 1998 Pan-American Workshop on Commercialization of Advanced Oxidation Technologies, London, Ontario, Jun 27th - 30th **1998**.

36. M. I. Stefan, J. R. Bolton, A. Safarzadeh-Amiri, J. Mack, S. R. Cater and B. W. Dussert, "Degradation Pathways during the Phototreatment of Methyl-*tert*-Butyl Ether by the UV/H_2O_2 Advanced Oxidation Process", IUPAC Symposium on Photochemistry, Barcelona, Spain, Jul 19th - 24th **1998**.

37. J. Mack and M. J. Stillman, "Magnetic Circular Dichroism Spectroscopy of Metal Phthalocyanine and Metal Porphyrin Anion Radical Species", First International Conference on Porphyrins and Phthalocyanines, Dijon, France, Jun 25th - 30th **2000**.

38. J. Mack, T. Nyokong and M. J. Stillman, "Magnetic Circular Dichroism Spectroscopy and INDO/s Calculations of Ruthenium Phthalocyanine", Second International Conference on Porphyrins and Phthalocyanines, Kyoto, Japan, Jun 30th - Jul 5th **2002**.

39. J. Mack, S. P. Keizer, B. Bench, S. Gorun and M. J. Stillman, "Optical Spectroscopy and electronic structure of 1,4,8,11,15,18,22,25-octafluoro-2,3,9,10,16,17,23,24-octaperfluoroisopropyl zinc phthalocyanine", Third International Conference on Porphyrins and Phthalocyanines, New Orleans, Louisiana, Jul 11th - 16th **2004**.

40. M. J. Stillman, J. Mack, C. Vermeiren and D. E. Heinrichs, "Characterization of heme scavenging pathogen cell wall proteins by MCD and ESI-MS techniques", Third International Conference on Porphyrins and Phthalocyanines, New Orleans, Louisiana, Jul 11th - 16th **2004**.

41. C. L. Vermeiren, S. E. Dale, J. Mack, M. J. Stillman and D. E. Heinrichs, "Characterization of iron-regulated surface determinants from *Staphyloccocus aureus*", 11th International Symposium on Staphylococci and Staphylococcal Infections. Charleston, SC. Oct 24th - 27th **2004**.

42. J. Mack, S. P. Keizer, B. Bench, S. Gorun and M. J. Stillman, "Optical Spectroscopy and electronic structure of 1,4,8,11,15,18,22,25-octafluoro-2,3,9,10,16,17,23,24-octaperfluoroisopropyl zinc phthalocyanine", The 2nd International COE Symposium, Sendai, Japan, Nov 22nd - 23rd **2004**.

43. M. J. Stillman, J. Mack, M. Pluym, C. Vermeiren and D. E. Heinrichs, " Magnetic circular dichroism study of the heme scavenging Isd proteins of *Staphylococcus aureus*", 12th International Conference on Biological Inorganic Chemistry, Ann Arbor, Michigan, Jul 31st - Aug 5th **2005**.

44. J. Mack, N. Kobayashi and M. J. Stillman, "MCD spectroscopy and TD-DFT calculations of Metal Porphyrinoids", 12th International Conference on Biological Inorganic Chemistry, Ann Arbor, Michigan, Jul 31st - Aug 5th **2005**.

45. J. Mack, N. Kobayashi and M. J. Stillman, "MCD spectroscopy and TD-DFT calculations of metal phthalocyanine anion and cation radical species" Fourth International Conference on Porphyrins and Phthalocyanines, Rome, Italy, Jul 2nd - 7th **2006**.

46. M. Pluym, C. L. Vermeiren, J. Mack, D. E. Heinrichs and M. J. Stillman, "Spectroscopic study of the Isd heme-scavenging proteins IsdA and IsdE of *Staphylococcus aureus*." Fourth International Conference on Porphyrins and Phthalocyanines, Rome, Italy, Jul 2nd - 7th **2006**.

47. A. Senior, J. Mack, N. Kobayashi and M. J. Stillman, "-cation radical porphyrinoids: Progress towards the assignment of the optical spectrum." Fourth International Conference on Porphyrins and Phthalocyanines, Rome, Italy, Jul 2nd - 7th **2006**.

48. C. L. Vermeiren, M. Pluym, J. Mack, D. E. Heinrichs and M. J. Stillman, "Characterization of the heme binding properties of iron-regulated surface determinant A (Isd A) from *Staphylococcus aureus*" Biometals 2006, Portland, Oregon, Jul 30th - Aug 6th **2006**.

49. W. Chidawanyika, S. Shimizu, J. Mack, N. Kobayashi and T. Nyokong, "Innovations in the development of low symmetry phthalocyanine derivatives", Fifth International Conference on Porphyrins and Phthalocyanines, Moscow, Russia, Jul 6th - 11th **2008**.

50. M. Kon-no, J. Mack, N. Kobayashi and T. Shinmyozu, "Electronic structures of tetrathiaporphyrin dication", 24th International Symposium on the Organic Chemistry of Sulfur, Florence, Italy, Jul 25th - 30th **2010**.

51. S. Sugawara, S. Kojima, Y. Yamamoto, J. Mack, N. Kobayashi, Z. Fu, K. M. Kadish, Y. M. Sung, K. S. Kim and D. Kim, "Synthesis, Characterization and Spectroscopic Analysis of Anti-aromatic 16 Benzofused Metalloporphyrin", Seventh International Conference on Porphyrins and Phthalocyanines, Jeju ICC, Korea, Jul 1st - 6th **2012**.

52. G. Kubheka, E. Amuhaya, J. Mack and T. Nyokong, "Synthesis, photophysical properties of hexabromoanilinoBODIPY dye-gold nanorods conjugate for use in Antimicrobial Photodynamic Therapy and TDDFT calculation of the aniline BODIPY dyes", The 17th SACI Inorganic Chemistry Conference, Grahamstown, South Africa, Jun 28th - Jul 2nd **2015**.

53. J. Stone, J. Mack and T. Nyokong, "Iodinated BODIPY dyes and their potential as photocatalysts", The 17th SACI Inorganic Chemistry Conference, Grahamstown, South Africa, Jun 28th - Jul 2nd **2015**.

54. M. Wildervanck, J. Mack and T. Nyokong, "Upconversion Nanoparticle-BODIPY conjugates for NIR activated singlet oxygen generation", The 17th SACI Inorganic Chemistry Conference, Grahamstown, South Africa, Jun 28th - Jul 2nd **2015**.

55. J. Stone, J. Mack and T. Nyokong, "Iodinated BODIPY dyes and their potential as photocatalysts", 6th Annual DST/Mintek NIC Workshop, Grahamstown, South Africa, Oct 28th - 29th **2015**.

56. M. Wildervanck, J. Mack and T. Nyokong, "Upconversion Nanoparticle-BODIPY conjugates for NIR activated singlet oxygen generation", 6th Annual DST/Mintek NIC Workshop, Grahamstown, South Africa, Oct 28th - 29th **2015**.

57. X. Liang, Y. Jiang, M. Li, J. Mack and W. Zhu, "Facile Modulation the Hydrogen Evolutions by A_2B Type Cu(III)Corroles Containing Different Fluoro-Atoms", Ninth International Conference on Porphyrins and Phthalocyanines, Nanjing, China, Jul 3rd - 8th **2016**.

58. X. Liang, Y. Jiang, M. Li, J. Mack and W. Zhu, "Halogenated A_2B type Co(III)corroles: Synthesis, Properties and Modulation Hydrogen Evolution Reactions", Ninth International Conference on Porphyrins and Phthalocyanines, Nanjing, China, Jul 3rd - 8th **2016**.

59. X. Liang, M. Li, J. Mack, N. Kobayashi and W. Zhu, "Synthesis and Electronic Structure of Zinc(II) Porphyrin Dimers with a Bridging Amide-Bonded Xanthene Moiety", Ninth International Conference on Porphyrins and Phthalocyanines, Nanjing, China, Jul 3rd - 8th **2016**.

60. T. Huang, X. Liang, M. Li, J. Mack and W. Zhu, "The First Example of Electrocatalyzed Full Dechlorination of DDT electrocatalyzed by Lipophilic Co(II)Pc", Ninth International Conference on Porphyrins and Phthalocyanines, Nanjing, China, Jul 3rd - 8th **2016**.

61. Dr John Mack, Dr Balaji Babu, Ms Rodah Soy, Mr James Oyim, Prof Edith Amuhaya, Prof Tebello Nyokong
    The use of Gaussian 09 to identify trends in the optical properties and electronic structures of porphyrin and BODIPY dye
    2018 CHPC National Conference, Cape Town, South Africa 2-6 Dec 2018