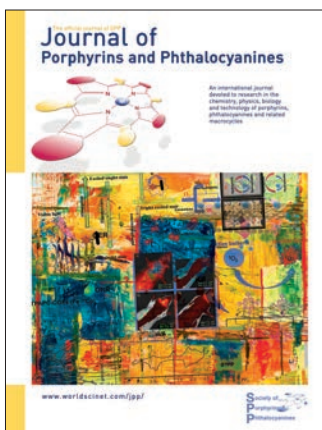


About the Cover



The cover shows a montage of the science presented in the current issue.

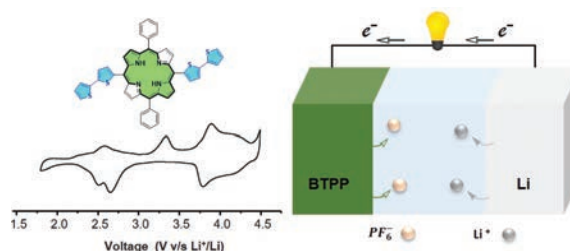
Articles

pp. 253–259

A bithiophene-substituted porphyrin displaying multi-electron redox processes as a cathode for lithium organic batteries

Shagor Chowdhury*, Saibal Jana, Svetlana Klayatskaya* and Mario Ruben*

5,15-di([2,2'-bithiophen]-5-yl)-10,20-diphenylporphyrin (BTPP) was synthesized and characterized. It was explored as a cathode material for lithium organic batteries. A discharge capacity of 128 mAh. g⁻¹ at a current density of 0.2 A. g⁻¹ with an average discharge voltage of 3.2 V was delivered. It showed a good rate capability upon cycling at different current densities. At a high current density of 10 A. g⁻¹, it delivered a discharge capacity of 32 mAh. g⁻¹.

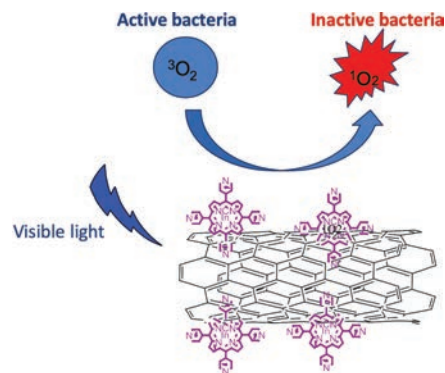


pp. 260–271

Photodynamic inactivation of *Staphylococcus aureus* and *Escherichia coli* with free-base and indium(III) 5,10,15,20-tetrakis(4-pyridyl) porphyrin adsorbed onto single-walled carbon nanotubes

N. Bridged Magaela, Mahlatse M. Ledwaba, Nonkululeko Malomane, John Mack, Tebello Nyokong* and Muthumuni Managa*

Adsorption of the porphyrin to SWCNTs was shown to have favorable aPDI activity when compared to free base and metalated porphyrins. The metalation and conjugation of porphyrins to SWCNTs improves their photophysical properties. Time-dependent density functional theory (TD-DFT) was used to establish a relationship between structural modifications to the porphyrin core, the resultant bathochromic shift and the intensification of the Q bands in the spectrum.



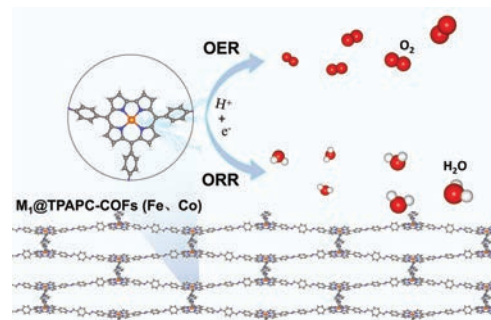
Articles

pp. 272–281

Theoretical screening of corrole-based covalent organic framework metal single-atom catalysts for ORR and OER

Yingjie Qu, Bin Li, Hangping Chen, Jin-Xia Liang*, Haiyan Wang* and Chun Zhu*

A series of stable metal corrole-based 2D monolayer single atom catalysts (SACs) written as $M_1@TPAPC-COFs$, where COF represents a corrole-based covalent organic framework, were obtained by screening using density functional theory (DFT) calculations. The calculations predicted two non-noble metal corrole-based 2D COF electrocatalysts, $M_1@TPAPC-COF$ ($M = Fe, Co$), with high electrocatalytic activity for ORR and/or OER.

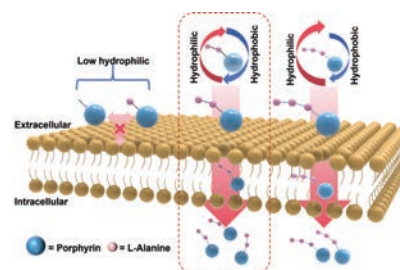


pp. 282–290

Regulating the *ct*DNA binding interactions and *in vitro* antitumor activities by chiral amide-bonded H₂Porphyrins containing zero- to three- L-alanine units

Wei Tang*, Ting Tang, Ting Yang, Jingkang Su, Huaijin Wang, Chaowen Shi*, Weihua Zhu and Xu Liang*

A series of four chiral amide-bonded free based porphyrins containing zero- to three- L-alanine units have tunable *ct*DNA bonding interactions and cell membrane penetration abilities that significantly enhance their antitumor behavior.

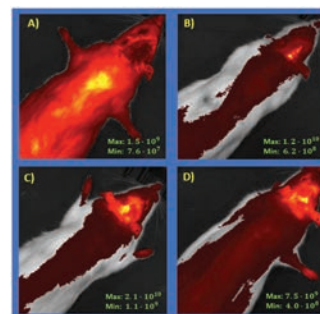


pp. 291–299

Pharmacokinetics of disulphonated tetraphenyl chlorin (fimaporfin/TPCS_{2a}) in a rat glioma model — methodology

Odrun A. Gederaas*, Mikael Lindgren, Kari Stigen, Anders Høgset and Henry Hirschberg

Using an orthotopic glioma rat model (F98 cells), the tumor localization and size are documented in the hippocampus by MRI and IVIS measurements. Results indicate no fluorescence in blood samples post 6 days after intravenous injection, but interestingly, a clear fluorescence was present in glioma *ex vivo* analyses 18 days after the cell instillation.

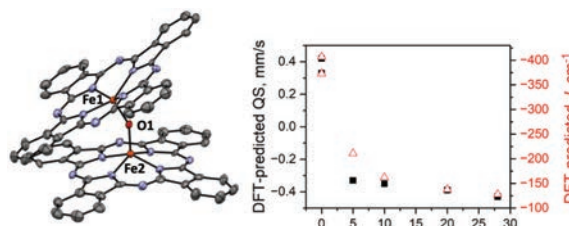


pp. 300–307

Finally: The X-ray crystal structure of the illusive unsubstituted iron(III) phthalocyanine μ -oxo(1) dimer. DFT-predicted Mössbauer quadrupole splitting and antiferromagnetic coupling constants for X-ray geometry

Victor N. Nemykin*, Nikolay N. Gerasimchuk and Breanna E. Muldowney

The structure of an illusive μ -oxo(1) isomer of $(PcFe)_2O$ complex, which has two antiferromagnetically coupled high-spin iron(III) centers and a bent Fe-O-Fe geometry is reported. DFT calculations were used to evaluate the antiferromagnetic coupling constant and Mössbauer quadrupole splitting in this compound.



Articles

pp. 308–317

Synthesis and characterization of porphyrin-MWCNT nanohybrid and its utilization as an antimicrobial agent against *S. aureus* and *E. coli*

Mohammad Tasleem, Pankaj Kumar Chaudhary, Ramasare Prasad and Muniappan Sankar*

A nanohybrid composed of porphyrin and MWCNT was synthesized and characterized by various spectroscopic and microscopic techniques. The nanohybrid exhibited excellent antibacterial activity against *E. coli* and *S. aureus*.

