Science and Engineering Research Board, Department of Science & Technology
(DST-SERB)

Theoretical investigation of porphyrin nanotubes for photodynamic and chemical sensor applications

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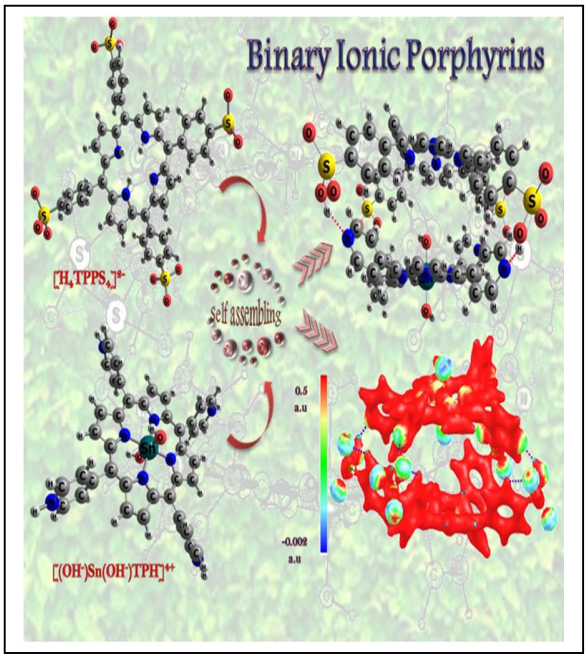
Amount Sanctioned: **Rs. 5,04,000/-** Year: **2014-2017**

Project outcomes:

- ✓ The structural and energetics of tetrakis(4-sulfonatophenyl) porphyrin diacid…Sn(IV)tetrakis(4-pyridyl) porphyrin (SnTP) metalloporphyrin layers such as $[H_4TPPS_4]^2$...$[SnTP]^{2+}$, $[H_4TPPS_4]^{2-}$...$[SnTPH]^{6+}$, $[H_4TPPS_4]^{2-}$...[X'SnXTP] and $[H_4TPPS_4]^{2-}$...$[X'SnXTPH]^{4+}$ (where X= X'= OH^-) were studied using quantum chemical techniques.
- ✓ The molecular patterns and interactions obtained for $[H_4TPPS_4]^2$...SnTPs show the importance of pyridine H atoms and axial ligands for the formation of perfect stack like complexes. The importance of pyridine H atoms is further inferred through formation of the slipped stack like structure of $[H_4TPPS_4]^{2-}$...X'SnXTPyP complex, which in-turn validates the formation of collapsed binary ionic porphyrin nanotubular structures.
- ✓ The existence of non-bonded interactions in the axially ligated binary ionic complexes analyzed through MEP maps and interaction energies further substantiate the functional dependence of porphyrin stacks on the substituents that are present.



Formation of binary ionic porphyrins stacks

- ✓ The reasonable stacking nature of $[H_4TPPS_4]^{2-}$...[X'SnXTP] complex in the presence of water molecules further supports the presence of solution around the layers for the formation of stable binary stacks. This work in general exhibits the formation of stack like $[H_4TPPS_4]^2$...SnTPs in the presence of axial ligand and pyridine protonation that might favor for the formation of hollow binary ionic porphyrin nanotubular structures.

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❖ **Publications:**

1. **G. Praveena** and A. Abiram, Structural and interaction properties of porphyrin Layers - A quantum chemical study, *Communications in Theoretical Physics,* 63: **2015,** 625–634.

2. J. Pavithra, A. Abiram and **G. Praveena,** Quantum chemical study on the structure and energetics of binary ionic porphyrin complexes, *Journal of Chinese Chemical Society,* 65: **2018**, 908-917.

❖ ***Conference/ Seminar/ Workshop:***

1. International conference on frontiers in nanoscience & nanotechnology at Sastra university, Thanjavur, Feb 26-28 (2016), Poster presentation: *"Structure and energetics of porphyrin nanoaggregate"*.

2. Theoretical Chemistry Symposium at Hyderabad, Dec 14-17(2016), Poster presentation: *"Theoretical study on binary ionic porphyrin nanoaggregates"*.

3. Virtual Winter School on Computational Chemistry *organized by Computational Chemistry team of Institute of Chemistry of High-Purity Substances, Russia; École polytechnique fédérale de Lausanne, Switzerland; Australian National University, Australia; Budapest University of Technology and Economics, Hungary; University of Victoria, Canada; University of Havana, Cuba; Université de Lille, France,* Jan 31-Feb 2(2018), Single File Presentation: *"Investigations on the structure and energetics of binary ionic porphyrins"*.

❖ Books: Nil

❖ Any other achievements:
