

Flow of Energy & Charge in Porphyrin Nanostructures

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Template-directed synthesis can be used to create π -conjugated nanostructures with sizes extending into the domain of proteins [1,2]. Do these systems mimic the light harvesting behavior of photosynthetic chlorophyll arrays [3]? Can electrons delocalize coherently around such large macrocycles? Do they display aromaticity [4]? Can tunneling through these nanorings result in quantum interference? This lecture will present progress towards answering these questions, including computational studies, such as the calculated map of nucleus independent chemical shift shown in Figure 1.

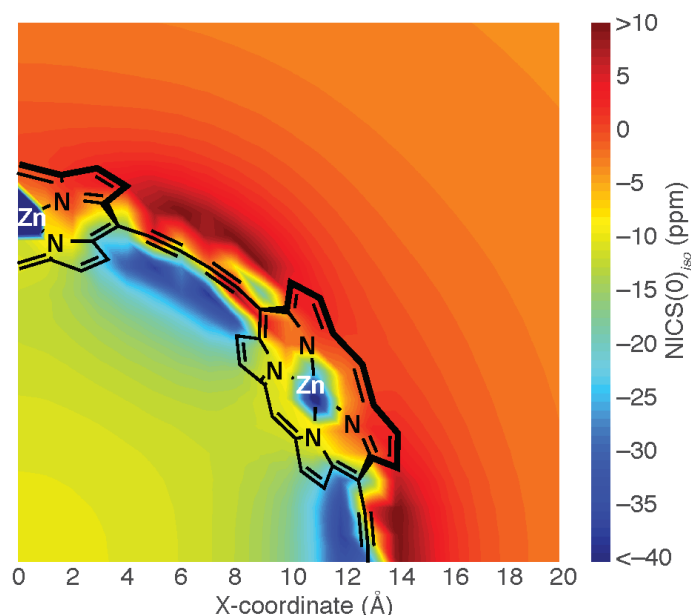


Figure 1. $\text{NICS}(0)_{\text{iso}}$ (B3LYP/def2-SV(P)) in the xy plane of a six-porphyrin nanoring in its 6+ oxidation state [4].

[1] M. C. O'Sullivan, J. K. Sprafke, D. V. Kondratuk, C. Rinfray, T. D. W. Claridge, A. Saywell, M. O. Blunt, J. N. O'Shea, P. H. Beton, M. Malfois, H. L. Anderson, *Nature*, **2011**, *469*, 72-75.

[2] D. V. Kondratuk, L. M. A. Perdigão, A. M. S. Esmail, J. N. O'Shea, P. H. Beton, H. L. Anderson, *Nat. Chem.*, **2015**, *7*, 317-322.

[3] C.-K. Yong, P. Parkinson, D. V. Kondratuk, W-H. Chen, A. Stannard, A. Summerfield, J. K. Sprafke, M. C. O'Sullivan, P. H. Beton, H. L. Anderson, L. M. Herz, *Chem. Sci.*, **2015**, *6*, 181-189.

[4] M. D. Peeks, T. D. W. Claridge, H. L. Anderson, *Nature*, **2017**, *541*, 200-203.