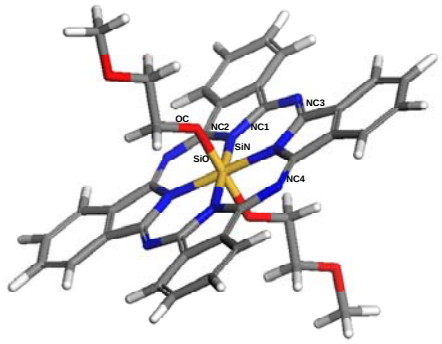
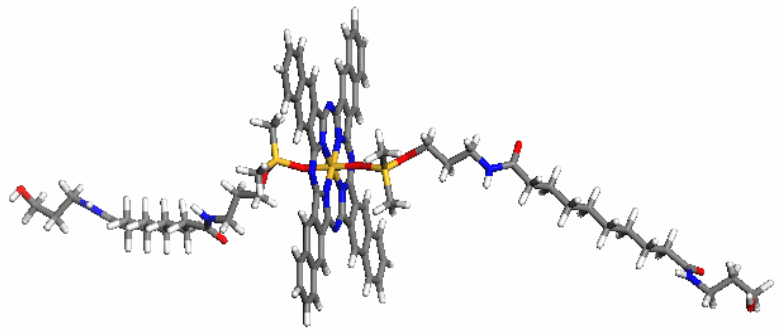
Optical Properties of Phthalocyanine and Naphthalocyanine Compounds

Jan Andzelm, Adam M. Rawlett, Joshua A. Orlicki, and James F. Snyder, U.S. Army Research Laboratory, and Kim K. Baldridge, University of Zurich, Zurich, Switzerland

Phthalocyanines (Pcs), naphthalocyanines (Ncs), and their derivatives are being used in numerous applications such as dyes and pigments, in photocopiers and printers, photovoltaic cells, gas sensors, nonlinear optical limiting devices, photodynamic therapy agents, and many other applications. These properties are the result of the stable macrocyclic conjugated network of π-electrons leading to high electrical polarizability and rapid nonlinear response of the charge density to the applied intense electromagnetic fields. The large nonlinear absorption in the visible spectrum, together with the ultrafast response time and easy processability, make the optical modulation abilities of this class of chromophores of key importance for many applications. The optical modulation properties of chromophores can be explained by a reverse saturable absorption (RSA) mechanism.

We have calculated optical properties of PCs and NCs complexes with Si as a central atom. We have confirmed that certain silicon- phthalocyanine and -naphthalocyanine compounds are strong RSA molecules. Results of this investigation improved our understanding of the role of axial substituents for Pcs and Ncs compounds and provided validation for the TDDFT approach that can be used for prediction of optical properties of numerous Ncs compounds. Additional, such studies can aid in synthetic possibilities for Ncs complexes having desirable optical properties.





Structure of $SiPc\text{-}(PEG_{75})_2$ SINC

Reference/Publication

Journal of Chemical Theory and Computation, 3, 870-877, **2007**