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Simulation of the electronic properties of Group 14 phthalocyanine derivatives

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Statement of the Problem: The focus of this project is to apply computational materials chemistry approaches to understand the ambipolarity of charge transport in crystalline Group 14 phthalocyanines. Such molecular materials, which fall under the broader context of organic semiconductors, are of interest for next generation, flexible electronics applications. More specifically, the project will deploy theoretical simulations run in a high-performance computing environment to provide evidence that the dimensionality of charge transport in these materials can be finely tuned by substituting the phenoxy axial groups with fluorine atoms and by varying their number of positions. In this step of the data collection process, the theoretical simulations were used to compute the energy values for different variations of phthalocyanine, internal reorganization energies, Huang-Rhys parameters for hole transport, and the shapes of the molecular orbitals.

Note : This work was partially published at International Conference on Bioinformatics & System Biology; March 20-21, 2019; Singapore City, Singapore