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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.

Biography

Asare Nkansah is an undergraduate student attending the University of Kentucky. He's in his fourth and final year with an intention of obtaining his bachelor's in computer science. During the first two years of his bachelor's degree, he conducted research in the nanoscience and computational facilities at Argonne National Laboratory. His experience with the Department of Energy assisted him in obtaining an opportunity overseas at the University of Bordeaux in France this previous summer. Over the course of three months in France, he focused his efforts on the field of theoretical-based chemistry-utilizing his computational skill set to model simulations that can predict the charge transport characteristics of phthalocyanine crystals.

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