First-Principles Calculations of the Electronic Structure of Single-Layer Naphthalocyanine Molecules

Adrian Bahri[†], Yu He[§], Chunjing Jia[†]

[†]*Department of Physics, University of Florida, 2001 Museum Rd, Gainesville, FL 32611*

[§]*Applied Physics and Physics Department, Yale University, 217 Prospect St, New Haven, CT 06511*

Recently organic molecules have found extensive application in the fields of molecular optics and molecular electronics due to their useful optical and electronic properties and their high degree of tunability. Among such molecules, phthalocyanine and its derivatives, especially naphthalocyanine (Nc), have become increasingly popular for study and application, though little has been done to study the electronic properties of a metal-free Nc monolayer. Here we report on the electronic properties of a metal-free Nc monolayer as well as a Nc monolayer adsorbed onto a substrate of Ag(100). First-principles calculations were performed in order to find the band structure, charge density, and density of states of both structures. These results allow us to characterize specific ways in which the substrate modifies the electronic properties of the molecular layer, such as a shift in band energies relative to the Fermi energy and introduction of dispersive bands through hybridization of C and Ag orbitals. We also characterize some differences between the orbitals of dispersive and non-dispersive bands in the Nc monolayer. A better understanding of the electronic properties of Nc and how they are modified by a substrate will allow for a greater ability to precisely tune the properties of novel materials and molecular electronics.