

Abstract Submitted
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Adsorption of Naphtho-Spiropyran On A Graphene Substrate LUCAS BROWNING, ANDREAS RIEMANN, Western Washington University — Spiropyran is a photochromic molecule that has been studied extensively for its applications in high density optical storage, optical switching, image processing and display. Spiropyran is a three-dimensional molecular switch which can be converted to Merocyanine, a planar isomer of Spiropyran where the central C-O bond has been broken. We are specifically studying the two isomers Naphtho-spiropyran and Naphtho-merocyanine adsorbed on a graphene substrate using computational chemistry methods with a combination of DFT and molecular mechanics. DFT is used to find the charge distribution and configuration while molecular mechanics is used to find the binding energy and adsorption geometry. With computational chemistry methods we found adsorption energies and inter-molecular adsorption geometries for the Spiropyran molecule on graphite. A similar approach is carried out for various Merocyanine isomers.

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