

Electronic and Optical Properties of Benzylpiperazine/CuI(111) System

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We present results of analysis of possible mechanisms responsible for the recently observed [1] strong orange fluorescence of Benzylpiperazine (BZP) molecules adsorbed on a CuI thin film. To evaluate the electronic structural properties of CuI(111) film, we carry out first-principles calculations based on Density-Functional Theory with the Generalized-Gradient Approximation using PBE exchange correlation functional along with the Hubbard Parameter (U). In particular, we examine the band structure and electronic density of states of the CuI film with the lowest energy, (111), geometry and that with defect states. We also calculate the excited states of the BZP molecule using time dependent density functional theory. We find that while the two parts of the system, CuI slab and BZP molecule, are individually optically in-active in the specific energy window, they produce strong visible light emission when coupled together. We trace the reason for such emission to optical transitions between the excited states of the molecule and the CuI(111) surface states. We discuss possible applications of the effect and that of defect states on other optical properties of the system, including excitonic effects.

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[1] R. Blair, unpublished.