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Optical properties of Benzylpiperazine/CuI (111) system[1] TAKAT RAWAL, VOLODYMYR TURKOWSKI, Physics Department and NSTC, University of Central Florida, RICHARD BLAIR, Department of Chemistry and Forensic Science Center, University of Central Florida, TALAT S. RAHMAN, Physics Department and NSTC, University of Central Florida — We are interested in understanding the mechanism responsible for the recently observed [1] strong orange fluorescence in systems that contain Benzylpiperazine (BZP) molecules adsorbed on CuI film. To study possible optical transitions we use ab-initio electronic structure calculations based on density functional theory with the generalized-gradient (PBE) approximation for the exchange-correlation functional. In particular, we examine in detail the band structure including defect states of the CuI film with the lowest energy (111) surface and the excited states of the BZP molecule. It is shown that while optically non-active in the corresponding energy window, the two parts of the system, CuI slab and BZP, produce strong visible light emission when coupled together. Our numerical analysis demonstrates that the reason for such emission is the optical transitions between the excited molecule and the iodine vapor atom states on the CuI (111) surface. We discuss possible applications of the effect and that of defect vapor atom states on other optical properties of the system, including excitonic effects in the ultrafast response. [1] R. Blair, unpublished.

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