

Investigating Aggregation and Excited State Dynamics During Deposition of a Phthalocyanine:Fullerene System

Nicholas M. Frainey,^{1,*} Zachary S. Walbrun,¹ and Cathy Y. Wong^{1,2}

¹Department of Chemistry and Biochemistry, University of Oregon, Eugene, Oregon, USA

²Oregon Center for Optical, Molecular, and Quantum Science, and Material Science Institute, University of Oregon, Eugene, Oregon, USA

*nfrainey@uoregon.edu

Abstract: This study seeks to illuminate the aggregation and excited state dynamics of intercalated phthalocyanine:fullerene thin films during deposition via *in situ* UV-vis spectroscopy and a spatially encoded transient absorption (TA) spectroscopy. © 2023 The Authors.

1. Introduction

Recently, copper phthalocyanine (CuPc) has become widely studied for optoelectronic applications due to its unique optical and electronic properties coupled with high degrees of thermal and chemical stability [1,2]. CuPc is a cheap commercial dye which forms pyramidal nanoribbon meshes with high surface coverage when solubilized in trifluoroacetic acid (TFA) and thereafter cast as a thin film [1,2]. When cast atop CuPc, the model electron acceptor material [6,6]-phenyl C₆₁ butyric acid methyl ester (PCBM) is shown to fill the void spaces throughout the CuPc nanomeshes [3], increasing the donor-acceptor interfacial area which may have promising applications in organic photovoltaics. Traditional spectroscopic measurements of CuPc and CuPc:PCBM have been conducted in solution and film phases; this work instead employs electronic spectroscopies during film deposition. We utilize *in situ* absorbance spectroscopy to draw insight regarding the molecular aggregation and concurrent single-shot transient absorption (SSTA) measurements to probe the excited-state behavior during the solvent evaporation process.

2. Experimental and Results

Solutions of 0.17 mg/mL CuPc in TFA and 2.96 mg/mL PCBM in chloroform were dropcasted onto glass slides on an electric hot plate with a slit in the middle, which permitted light to pass through for concurrent absorbance and SSTA measurements to be taken as the films dried. Absorbance spectra for dry films of CuPc deposited on PCBM and PCBM deposited on CuPc (Fig. 1a) show differences in electronic structure based on the order of layers. *In situ* absorbance measurements during CuPc deposition (Fig. 1b) show an intermediate phase with a feature centered at 608 nm, and concurrent SSTA measurements show high TA signal during this intermediate phase.

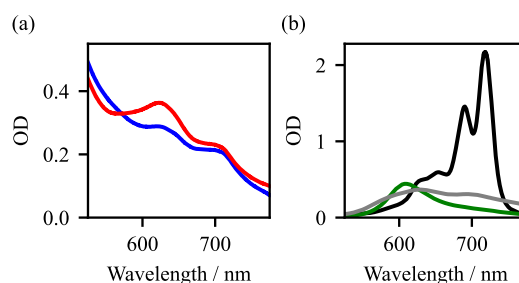


Fig. 1. (a) Absorbance spectra for dry thin films of PCBM deposited atop CuPc (red) and CuPc deposited atop PCBM (blue). (b) *In situ* absorbance spectra showing CuPc in solution (black), in the intermediate phase (green), and as a dry film (gray).

3. Acknowledgements

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4. References

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