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Thin Film Organic Solar Cells: Theoretical and Experimental Band Gap Energy Calculations.¹ SHELBY DAVIS, STEPHEN PORTER, JERRY CHAMNICHANH, JULIA D'ROZARIO, State University of New York at Oswego, ZAHRA AHMADI, JACK RODENBURG, University of Nebraska at Lincoln, LUCIE ROUTABOUL, University of Strasbourg, France, AXEL ENDERS, Universitt Bayreuth, Germany, PETER DOWBEN, University of Nebraska at Lincoln, CAROLINA C. ILIE, State University of New York at Oswego, UNIVERSITY OF NEBRASKA AT LINCOLN TEAM, STATE UNIVERSITY OF NEW YORK AT OSWEGO TEAM — We analyze here different organic thin films with potential use for solar cells. We calculate the molecular orbitals and we obtain the band gap. We notice that the added zwitterions diminish the band gap of the film, making better solar cells. The two solar cells are obtain by depositing on the substrate of choice two different polymers, polyaniline and poly(3-hexylthiophene-2,5-diyl), and the zwitterion: p-benzoquinone monoamine. The band gap is theoretically calculated by using HyperChem package and obtained experimentally via Halogen and Deuterium spectra measurements. The I-V curves show that these films have great potential as efficient solar cells, as shown by the calculated ideality factor.

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