Abstract Submitted for the MAR06 Meeting of The American Physical Society

Hückel theory of large-scale planar organic structures WILLIAM SCHWALM, University of North Dakota, MIZUHO SCHWALM, University of Minnesota-Crookston — Hückel theory applies, if at all, to the π orbitals of planar organic molecules, treating only one p_z -like basis function for each atomic site. The only advantage of this is that one has closed formulas for properties of rather large, complex structures. We develop π -orbital Green function calculations for \vec{k}_{\parallel} resolved density of states of ordered layers of organic adsorbates, such as might pertain to angle-resolved photoemission. Simple-minded though it may be, the theory leads to closed formulas for a wide variety of molecular architectures.

William Schwalm University of North Dakota

Date submitted: 29 Nov 2005

Electronic form version 1.4