

Abstract Submitted  
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**On the theory of Carriers's Electrostatic Interaction near an Interface** MICHAEL WATERS, HOSSEIN HASHEMI, JOHN KIEFFER, Univ of Michigan - Ann Arbor — Heterojunction interfaces are common in non-traditional photovoltaic device designs, such as those based small molecules, polymers, and perovskites [1]. We have examined a number of the effects of the heterojunction interface region on carrier/exciton energetics using a mixture of both semi-classical [2] and quantum electrostatic methods, *ab initio* methods, and statistical mechanics. Our theoretical analysis has yielded several useful relationships and numerical recipes that should be considered in device design regardless of the particular materials system. As a demonstration, we highlight these formalisms as applied to carriers and polaron pairs near a C60/subphthalocyanine interface [1]. On the regularly ordered areas of the heterojunction, the effect of the interface is a significant set of corrections to the carrier energies, which in turn directly affects device performance.

[1] S.E. Morris et al, Organic Electronics, Vol. 15, 12, 2014

[2] J. D. Jackson, Classical Electrodynamics, 1962.

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