

# Photo-Induced Open Circuit Voltage in Graphene-Based Organic Photovoltaics and Its Origin

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## Abstract

We investigated the origin of open circuit voltage in graphene-based organic photovoltaics (OPVs) from I-V measurements at 1 Sun irradiation and using Kelvin Probe Force Microscopy (KPFM) under laser illumination. In this work we utilized poly(3-hexyl-thiophene):phenyl-C<sub>61</sub>-butyric acid methyl ester (P3HT:PCBM) blend as a photoactive layer to fabricate bulk heterojunction OPVs. Our experiments demonstrated that thin P3HT:PCBM OPVs assembled on transparent graphene electrodes exhibit higher open circuit voltages ( $V_{oc} \approx 0.79 \pm 0.01$  eV) than identical ITO-based OPVs ( $V_{oc} \approx 0.60 \pm 0.01$  eV). Both previously reported models, the band energy offset [1] and the metal-insulator-metal models [2], failed to explain the high open circuit voltage in graphene-based OPVs. Using KPFM under illumination, we found that the work function of graphene thin film electrodes strongly increase with increasing intensity of illumination and the amounts of photoexcited holes injected into graphene, as shown schematically in Figure 1. This result led us to propose a dynamic graphene-insulator-metal model (d-GIM) based on the specific zero-band gap semiconducting properties of graphene. Our d-GIM model predicts an open circuit voltage of  $V_{oc} = 0.74$  V for thin graphene-based OPVs that compares well with the value of  $V_{oc} = 0.79 \pm 0.01$  V directly measured from I-V curves. Our d-GIM model sheds light on the factors that influence controlling the open circuit voltage in virtually any ultrathin OPVs. Since the efficiency of OPVs is proportional to the open circuit voltage, our findings can be seen as a critical step towards improving the performance of organic photovoltaics.

## References

[1] B. P. Rand, D. P. Burk, S. R. Forrest, Phys. Rev. B, 11 (2007), 115327: 1-11.

[2] V. D. Mihailetschi, P. W. M. Blom, J. C. Hummelen, and M. T. Rispens, J. Appl. Phys., 10 (2003), 6849–6854.

## Figures

Figure 1: Schematic of hole generation and Fermi level shift in graphene-based solar cells under illumination. The shift in the Fermi level and the subsequent increase in the work function of graphene lead to larger difference between the work function of Al top contact and graphene electrode. This difference corresponds to the open circuit voltage.

