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Effect of conjugation linkage in molecular dipolar phosphonic acids for modification of zinc oxide in organic photovoltaics JENNIFER BRAID, NREL, Colorado School of Mines, SARAH COWAN, BRAD MACLEOD, NREL, UNSAL KOLDEMIR, ALAN SELLINGER, REUBEN COLLINS, TOM FURTAK, Colorado School of Mines, DANA OLSON, NREL — Self assembled monolayers of small molecules have become popular to modify the physical and electronic properties of metal oxide and conductive contacts for use in organic and hybrid electronics. Here, we discuss the application of phosphonic acid interface modifiers with strong molecular dipole moments that are able to effectively tune the work function of zinc oxide. This effect is exploited in organic photovoltaic devices, where decreasing the work function of the electron transport layer relative to the LUMO level of the active layer electron acceptor translates to an increased open circuit voltage. However, the effect of the molecular dipole moment is only part of the story, as we have found that bond type within the phosphonic acid also plays a role in the work function shift. Zinc oxide modified with 2,6-difluorophenylvinylphosphonic acid and its nonconjugated counterparts was studied via Kelvin probe and IR spectroscopy, as well as in P3HT:ICBA inverted devices, revealing that the conjugated double bond dramatically accentuates the aforementioned change in work function, resulting in improved device performance relative to the unconjugated modified or the un-modified ZnO contact.

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