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Improving Band Line-up: DFT study of interface effects MICHELLE TOMASIK, MIT Physics, DAVID STRUBBE, MIT Materials Science and Engineering, ALEXIE KOLPAK, MIT Mechanical Engineering, JEFFREY GROSSMAN, MIT Materials Science and Engineering — Solar cells, organic light emitting diodes, and other devices that involve organic molecules require metal contacts to either extract or supply electricity. Unfortunately standard band-line-up diagrams fail to include important interface effects. Using density functional theory (DFT), we studied metal/organic interfaces to probe the different interface effects, including image charge interactions and dipoles arising from various sources at the interface, and predict how they will affect the line-up of the energy levels. Specifically we have looked at two very different organics, Alq3 and anthracene on different metals.

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