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DFT study of metal/organic interfaces; optimizing morphology and energy levels for maximum Voc MICHELLE TOMASIK, ALEXIE KOLPAK, JEFFREY GROSSMAN, MIT — Metal/organic interfaces are important for understanding the electronic properties of any device incorporating organic molecules, although these interfaces have been much less studied than their metal/inorganic counterparts. Using density functional theory, we examine the electronic structure of the interfaces of three metals: silver, aluminum, magnesium, and an organic molecule, Alq3, which is utilized in organic light emitting diodes. We calculate properties of interfaces with a clean metal surface as well as ones with small metal particles injected close to the organic. The effects of the different metals are to charge the Alq3 to varying degrees and perturb the energy levels as the metal states mix with the organic molecule. Insights into the energy level alignment and morphology at these interfaces as a function of the electrode workfunction will be discussed, with the goal of maximizing the open circuit voltage through the choice of metal and deposition process.

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