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Quasiparticle Gaps of Nanostructures Weakly-Coupled to their Environments: The Case of C60/Metal Interfaces[1] JAY SAU, Department of Physics, U C Berkeley, Material Science Divsion, LBNL, JEFFREY NEATON, Molecular Foundry, LBNL, HYOUNG-JOON CHOI, Department of Physics and IPAP,Yonsei University, Korea, STEVEN G. LOUIE, MARVIN L. COHEN, Department of Physics, U C Berkeley, Material Science Divsion, LBNL — A new approach based on density functional theory is developed to calculate charging energies and quasiparticle energy gaps of molecular systems weakly-coupled to an external environment. The approach is then applied to the case of a C60 molecule adsorbed on the Au(111) and Ag(100) surfaces. For C60/Au(111), the calculated quasiparticle gap is reduced by 2.34 eV relative to the gas-phase, consistent with recent experiments. For the more strongly-coupled C60/Ag(100) system, the predicted gap is also reduced, but differs from experiment by 0.5eV. The discrepancy is identified as being due to screening due to charge transferred from the metal to the molecule and is resolved by solving an effective Anderson Hamiltonian within the GW approximation for the carriers in the HOMO and LUMO states, which results in an extra renormalization of the gap for the Ag(100) case.

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