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The evolution of molecule-electrode coupling at biased interfaces: An ab initio approach ZHENFEI LIU, JEFFREY B. NEATON, Lawrence Berkeley National Laboratory — Coupling of discrete molecular states to a metallic continuum at an interface, together with level alignment between frontier molecular orbital energies and the Fermi level, determine its transport and spectroscopic properties. In addition, phenomenological coupling parameters between the discrete molecular states and the continuum are necessary for understanding I-V characteristics and constructing models of charge dynamics at the interfaces. In this work, we compute such coupling parameters based on a non-equilibrium Green's function approach, and analyze the bias-induced change of such coupling parameters and their effect in transport properties and I-V characteristics. We study and compare a series of model interfacial systems, molecular junctions including bipyridine and its derivatives (both symmetric and asymmetric), under bias. Our study provides new understanding of finite bias transport properties in terms of molecular orbitals for such junctions, and new insight in interpreting experimental measurement of I-V characteristics.

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