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All Electron Calculations of IV Characteristics For Molecular Junctions JOHN LAWSON, CHARLES BAUSCHLICHER, NASA Ames Research Center — We present current-voltage (I-V) characteristics computed using all-electron basis sets on the conducting molecule. We consider benzene dithiol with gold contacts as our model system. The all-electron results are very similar to previous results obtained using effective core potentials (ECP). A hybrid integration scheme is used that keeps the all-electron calculations cost competitive with the ECP calculations. By neglecting the coupling of states to the contacts below a fixed energy cutoff, the density matrix for the core electrons can be evaluated analytically. The full density matrix is formed by adding this core contribution to the valence part that is evaluated numerically. Expanding the definition of the core in the all-electron calculations significantly reduces the computational effort and, up to biases of about 2 V, the results are very similar to those obtained using more rigorous approaches. The convergence of the I-V curve and the transmission function with respect to basis set is discussed.

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