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Semiconductor/Molecule Transport Junctions: An Analytic Form For The Self-Energies VLADIMIRO MUJICA, Research Professor, MARK RATNER, Professor — We have derived an approximate analytic expression for the spectral density of a simple model of a semiconductor/molecule junction. The semiconductor is considered as a tight-binding one-dimensional chain with periodic boundary conditions, and either bond or site-energy, alternation to mimic a two-band system. Using the simplest representation for an atomic or molecular site we obtain a spectral density whose main physical and mathematical features are independent of the alternation pattern. In this contribution, we show applications of our model to the description a variety of junctions where the relative position of the energy levels involved is changed.

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