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Electron Transfer Using Non-Orthogonal Basis Functions[1] TZU-CHENG WU, DAVID DUNLAP, Univ of New Mexico, STEVE VALONE, Los Alamos National Laboratory, SUSAN ATLAS, Univ of New Mexico — We reconsider standard models of electron transfer in molecular solids formulated with non-orthogonal wavefunctions characterized by weak coupling matrix element V and small wavefunction overlap S. Using the method of Weisskopf and Wigner, we derive a new expression for the phonon-assisted electron hopping rate (Marcus rate) between non-degenerate sites separated by energy difference Δ. We show that electron localization occurs for a particular value of the ratio $S\Delta/V$, and we discuss the implication this has for the Marcus inverted regime.

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