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Tunneling Transport through Long Molecular Chains[1] EMIL PRODAN, Department of Physics, Yeshiva University, New York, NY, ROBERTO CAR, Chemistry Department, Princeton University, Princeton, NJ — The Riemann structure of the bands and other properties of the evanescent Bloch functions have been used to derived an asymptotic expression for the tunneling conductance through long molecular chains. Our results give the contact conductance in terms of an overlap integral of three well defined and physically relevant quantities. In particular, this formula shows how the conducting states of the leads couple to the evanescent Bloch functions of the insulating chain. The theory is applied to amine-linked alkyl and aromatic chains and the results are compared with the experiment. Using these applications, we discuss the key aspects and advantages of the theory. Extensions to spin dependent transport will be also discussed.

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