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Thermoelectric transport parallel to the planes in a multilayered Mott-Hubbard heterostructure[1]

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We present a theory for charge and heat transport parallel to the interfaces of a multilayer (ML) of the ABA type, where A and B are materials with strongly correlated electrons. When separated, both materials are half-filled Mott-Hubbard insulators with large gaps in their excitation spectrum. In a ML, the renormalization of the energy bands gives rise to a charge reconstruction which breaks the charge neutrality of the planes next to the interface. The ensuing electrical field couples self-consistently to the itinerant electrons, so that the properties of the ML crucially depend on an interplay between the on-site Coulomb forces and the long range electrostatic forces. Using the Falicov-Kimball model, we compute the Green's function and the local charge on each plane of the ML by inhomogeneous DMFT and find the corresponding electrical potential from Poisson's equation. The self-consistent solution is obtained by an iterative procedure, which yields the reconstructed charge profile, the electrical potential, the planar density of states, the transport function, and the transport coefficients of the device. For the right choice of parameters, we find that a heterostructure built of two Mott-Hubbard insulators exhibits, in a large temperature interval, a linear conductivity and a large temperature-independent thermopower. The charge and energy currents are confined to the central part of the ML. Our results indicate that correlated multilayers have the potential for applications; by tuning the band shift and the Coulomb correlation on the central planes, we can bring the chemical potential in the immediate proximity of the Mott-Hubbard gap edge and optimize the transport properties of the device. In such a heterostructure, a small gate voltage can easily induce a MI transition. Furthermore, the right combination of strongly correlated materials with small ZT can produce, theoretically at least, a heterostructure with a large ZT.

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