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Real-space pseudopotential method for charge and spin transport properties of nanoscale junctions[1] LINGZHU KONG, University of Minnesota, JAMES R. CHELIKOWSKY, University of Texas at Austin, JEFFREY B. NEATON, The Molecular Foundry, Lawrence Berkeley National Laboratory, STEVEN G. LOUIE, University of California, Berkeley & Lawrence Berkeley National Laboratory — We present an *ab initio* method for the electronic transport of nano-scale junctions under finite bias. Our method is based on density functional theory using real space pseudopotentials. The scattering wave function is obtained by solving a set of linear equations with a sparse coefficient matrix. Our method does not require a matrix inversion. We apply the method to Na or Mg atomic point contacts coupled to two planar electrodes, and good agreement with previous work is obtained. We also extend this study and examine spin-dependent transport in select magnetic atomic point contacts, where trends in magnetoresistence are examined as a function of junction bias, magnetic moment, and electronic coupling.

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