Open boundary-conditions using empirical pseudopotentials in quantum transport\(^1\) BO FU, MASSIMO FISCHETTI, The University of Texas at Dallas — As device dimensions approach the 10 nm length-scale, the study of electronic transport requires the knowledge of an accurate band structure and of transport equations transcending the semiclassical Boltzmann picture. Having as our ultimate goal the study of dissipative quantum transport using the Pauli Master Equation, in this talk we address the numerical issue of how to formulate and implement numerically the open-boundary-condition Schrödinger equation within an empirical-pseudopotential full-band framework. Results regarding ballistic transport in Si nanowires will be presented.

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