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Source and sink approach to calculate transport properties of nanostructures KALMAN VARGA, SOKRATES PANTELIDES, Vanderbilt University — We have calculated the transport properties of single molecule and carbon nanotube devices using the the Source and Sink method. We have carefully tested the convergence of the current by enlarging the basis. The fully converged current-voltage characteristics presented in this paper can serve as benchmark for transport calculations. We also compare our results to those obtained by other approaches and analyze the source of disagreements.

Kalman Varga Vanderbilt University

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