Parallelized electronic transport calculations in real space
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KRONIK, Weizmann Institute of Science, Israel — We present a real-space method
for first-principles nano-scale electronic transport calculations, using the non-
equilibrium Green's function (NEGF) method and complex absorbing potentials
(CAPs) to represent the effects of the semi-infinite leads. In real space, the elec-
tronic Hamiltonian from Density Functional Theory (DFT) is very sparse. As a
result, the transport problem parallelizes naturally and can scale favorably with
system size. We illustrate our method with calculations on several realistic test
systems and find good agreement with a reference calculation.

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