A Planewave-based Method for First-Principles Electron Transport

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In this talk, I present a new method for studying complex band structure and electron transport across molecular and/or nano-junctions.
We implement this method in calculations based on the density functional theory using planewave basis set in conjunction with pseudo-potentials.
Starting with scattering theory, we derive the formalism and algorithms that solve the transmission/reflection coefficients for wave functions in 2D slice.
The total transmission and reflection coefficients across a 3D scattering region are obtained using a layer combination technique, which can be
effectively parallelized. I will demonstrate the calculated complex band for silicon and transmission coefficient through a vacuum.