



SI2-SSE: **PERTURBO**: a software for accelerated discovery of microscopic electronic processes in materials

Caltech

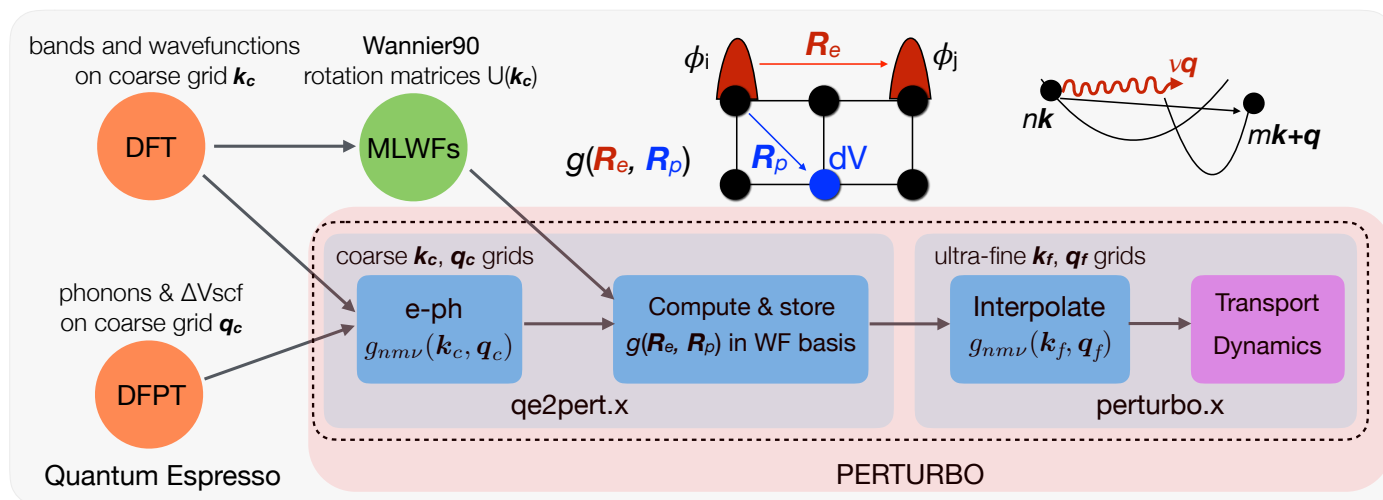
Award #: 1642443

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Why? “Understanding *dynamical processes* involving electrons, lattice vibrations (phonons), atomic defects, and light *in the solid state* is key to *advancing functional materials and next-generation devices*”

How? A platform for *ab initio* transport and dynamics in solids (hot carrier cooling, carrier conductivity, spin-flip dynamics)

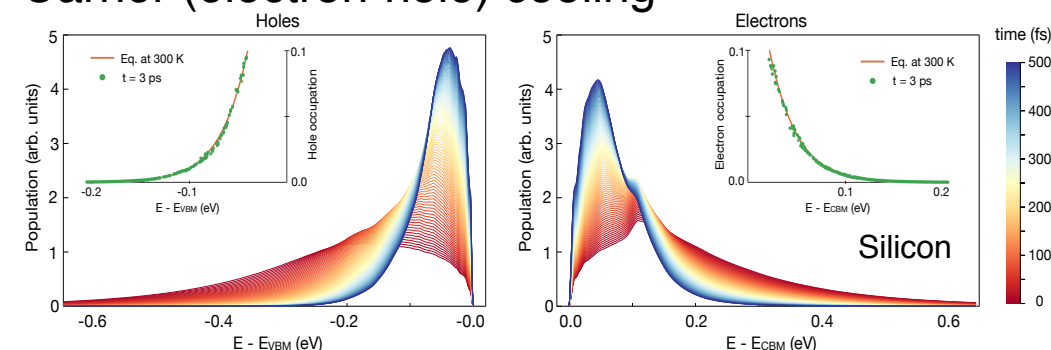
For example, PERTURBO e-ph interaction workflow



Related work and publications using PERTURBO, please see <http://bernardi.caltech.edu/publications/>

What? <https://perturbo-code.github.io/>

Carrier (electron-hole) cooling



Spin-flip dynamics (Elliot-Yafet mechanism)

