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

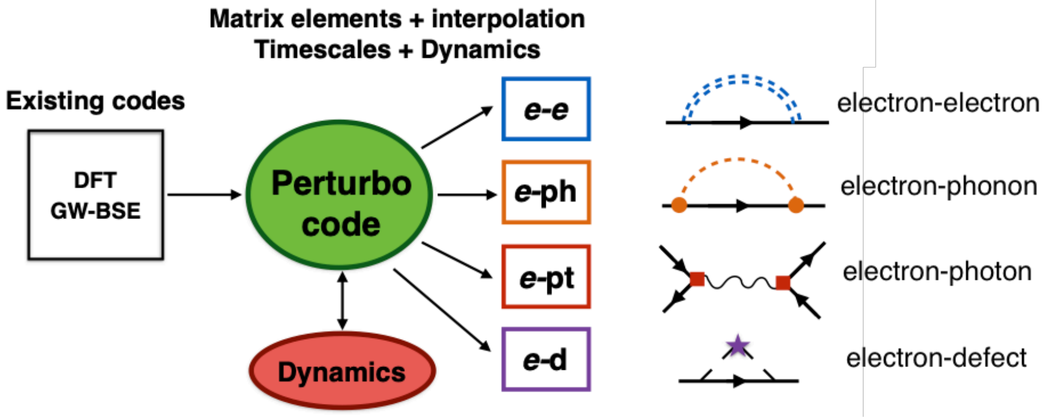
Award #: 1642443

Marco Bernardi (PI), I-Te Lu (presenter)

Department of Applied Physics and Materials Science, California Institute of Technology

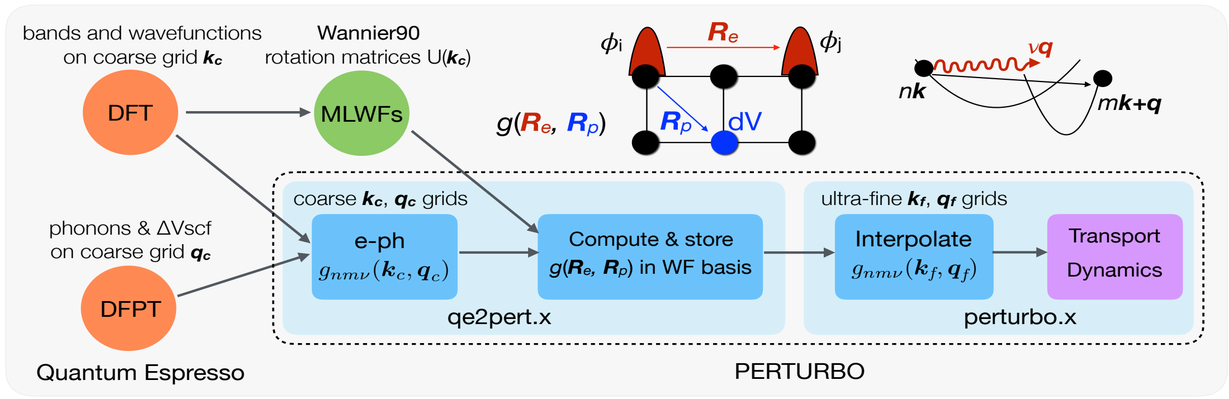
Background

- Solid-state technologies depend crucially on **charge carrier scattering and dynamics.**
- The dynamical processes involve the interactions of electrons with electrons, lattice vibrations (phonons),light (photons), and atomic defects.
- PERTURBO is a robust platform to study electron scattering processes using **first-principles calculations and many-body perturbation theory** with angstrom space and femtosecond time resolutions.

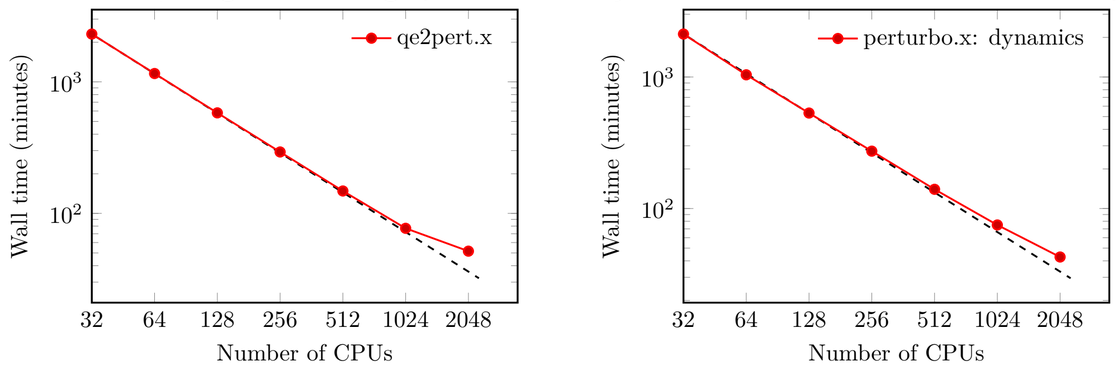


PERTURBO platform

- Current PERTURBO mainly supports e-ph interactions
- Subroutines for e-e, e-pt, and e-d interactions are in progress

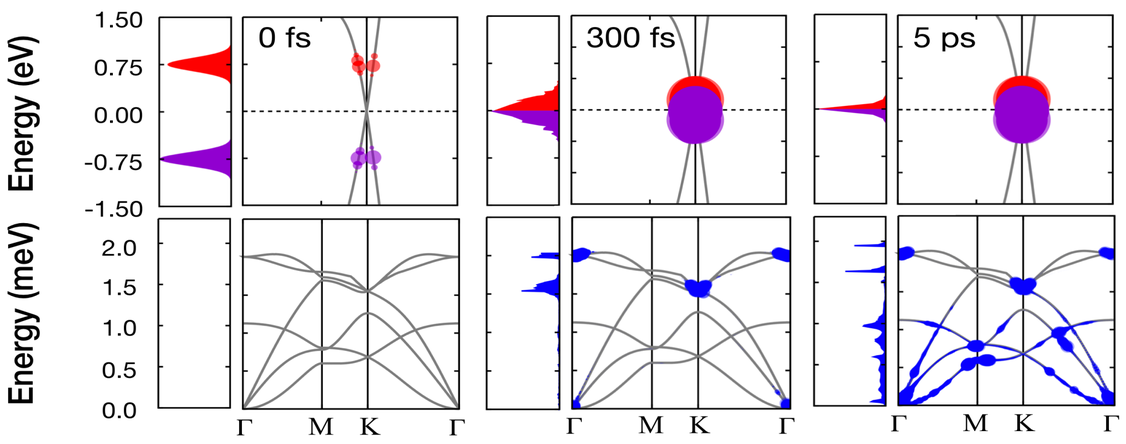


- Modern programming (HDF5 & hybrid MPI/OpenMP parallel)

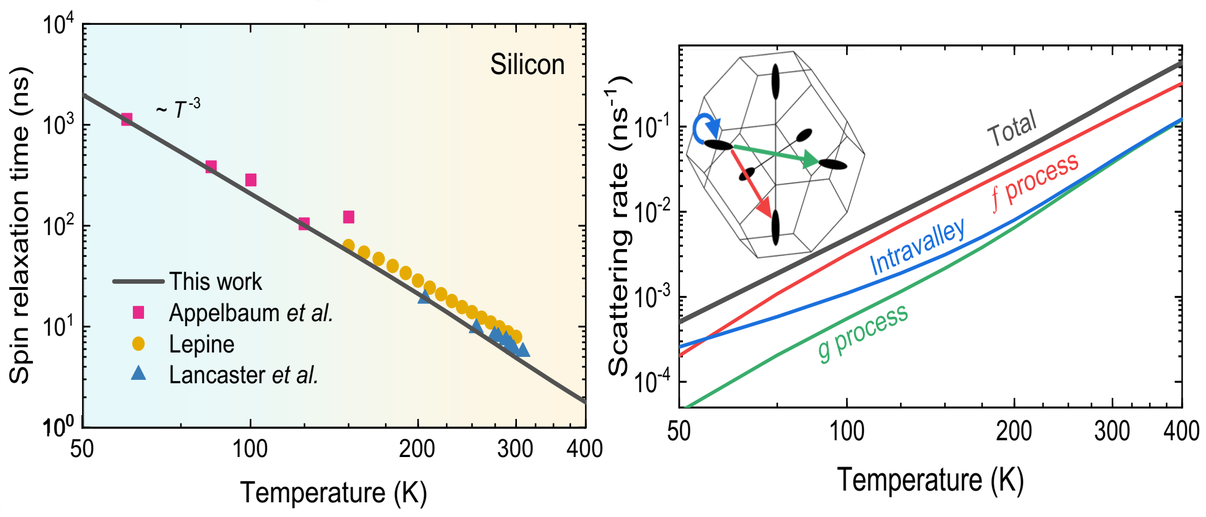


Carrier dynamics

- Hot carrier cooling and spin-flip dynamics can be modeled fully from first principles methods
- Time-step electron/hole & phonon occupations in graphene



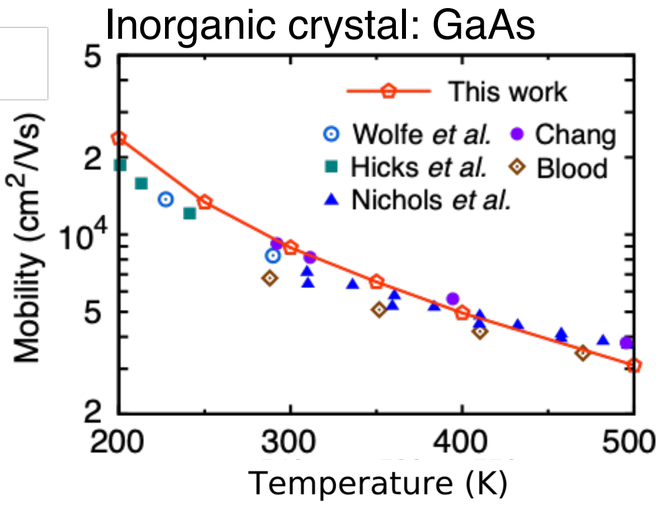
- Spin-flip dynamics and valley scattering mechanisms e-ph scattering flips electron spin (Elliot-Yafet mechansim)



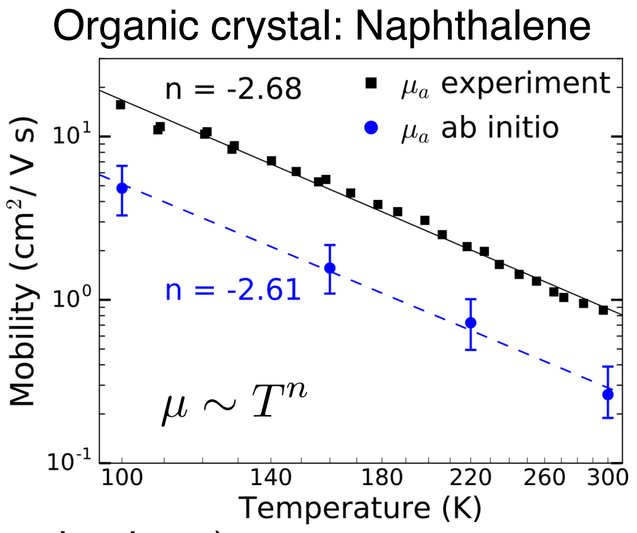
Charge transport

- Compute mobility based on Boltzmann transport equation
- Temperature and state-dependent relaxation time from first-principles

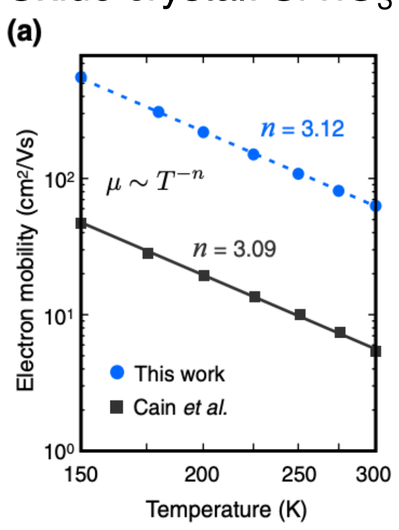
Inorganic crystal: GaAs

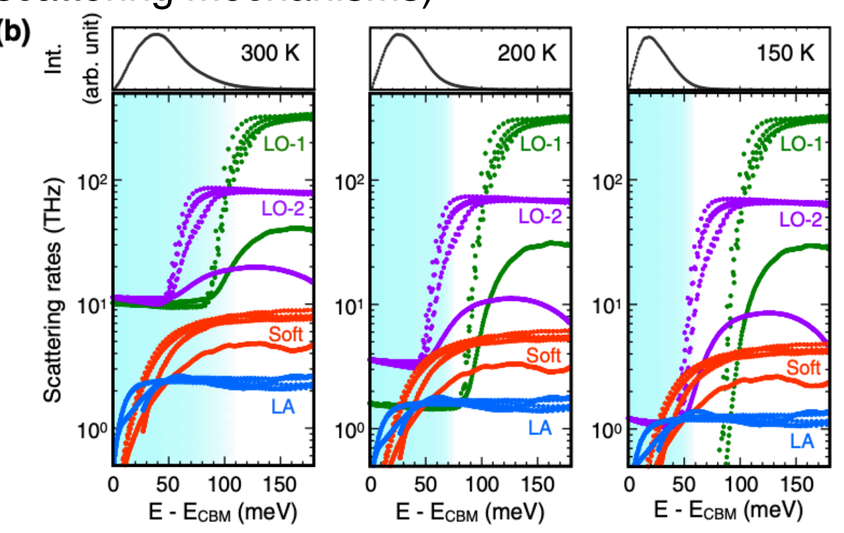


Organic crystal: Naphthalene



Oxide crystal: $SrTiO_3$ (scattering mechanisms)





As for references, please see Marco Bernardi group website (http://bernardi.caltech.edu/publications/) for more details

Our research model canvas (overview)

Key partners

We acknowledge

NSF · NERSC · JCAP Joint Center for Artificial Photosynthesis · XSEDE Extreme Science and Engineering Discovery Environment · Air Force Office of Scientific Research · Caltech

Key activities

- Develop main subroutines
- Maintain code website
- Organize workshop

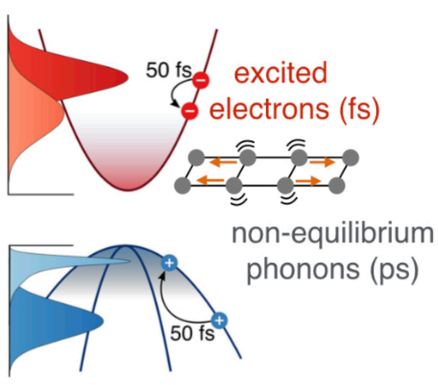
Key resources

- PERTURBO source codes
- Excellent postdocs and graduate students
- Computer resources

Value proposition

PERTURBO

- Compute charge transport and dynamics in solid-state materials from first principles methods



Customer relationship

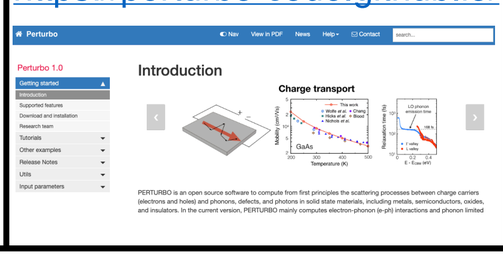
- Become a free member to access the source codes

perturbo@caltech.edu

Channel

PERTURBO website

https://perturbo-code.github.io/



Customer

- Scientists who work on first principles calculations
- Experimentalists who work on ultrafast dynamics
- Researchers who work on materials informatics
- Engineers who design new materials and devices

Cost structure

PERTURBO developer team in Marco Bernardi research group

Revenue stream

Users, Publications, Scientific discovery, Materials design