Studying Direct and Phonon-assisted Quantum Processes in Semiconductors

DOE CSGF Annual Review

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Kyle Bushick, Sieun Chae, Kelsey Mengle, Nocona Sanders, Zihao Deng, Emmanouil Kioupakis

Studying Direct and Phonon-assisted Quantum Processes in Semiconductors

Energy bands: allowed states for carriers

Band gap: energies with no allowed states between occupied and unoccupied bands

Dopability: ~10^{13}-10^{21} dopants / cm^3
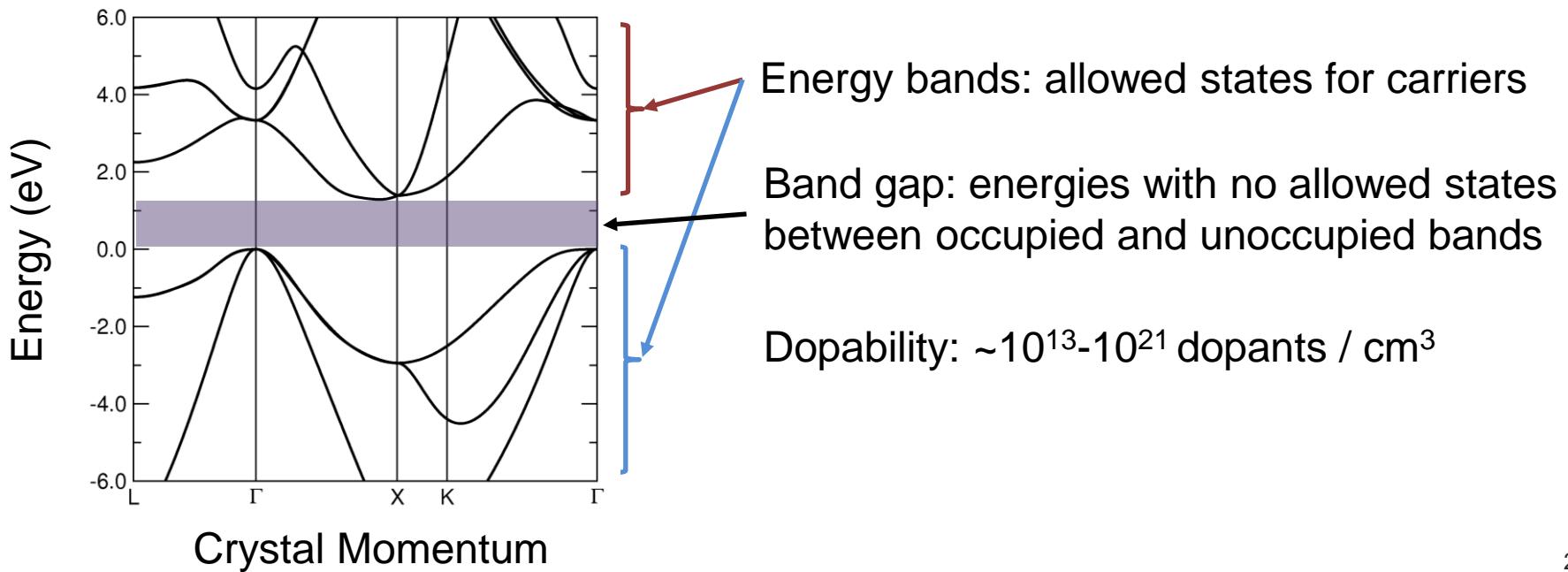
Studying **Direct and Phonon-assisted Quantum Processes** in Semiconductors

Direct

1-step

Transition between initial and final state

Energy and momentum conservation
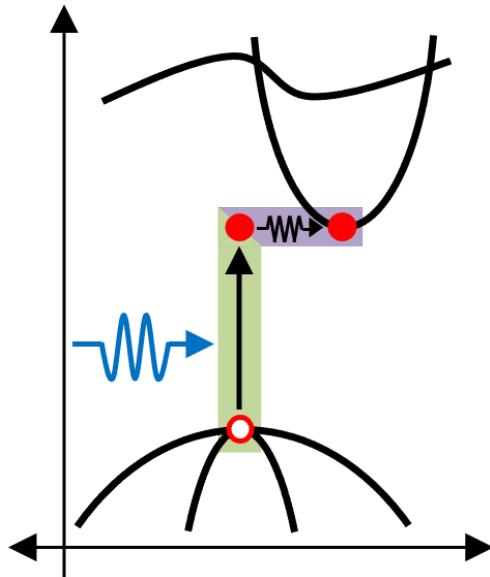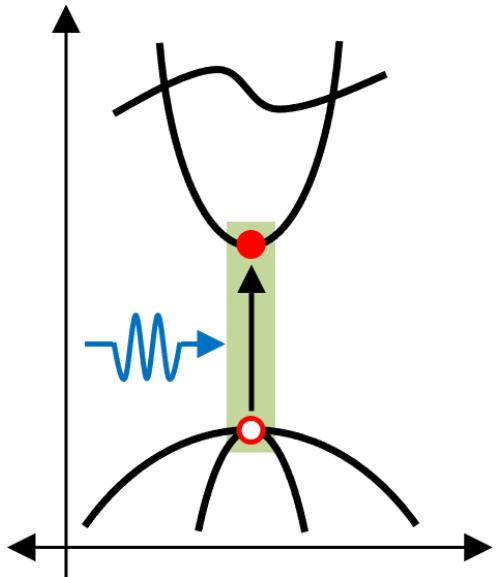
Phonon-assisted

2-step

Includes "virtual" transition with an intermediate state

Momentum conservation relaxed

From Macroscopic to Microscopic
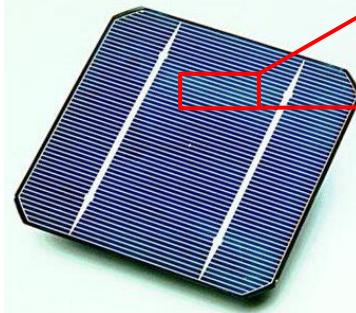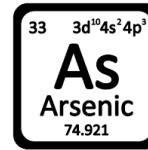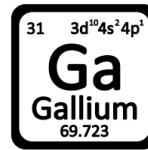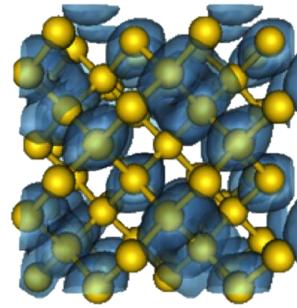
$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v_{KS}(\boldsymbol{r})\right)\varphi(\boldsymbol{r}) = \varepsilon\varphi(\boldsymbol{r})$$
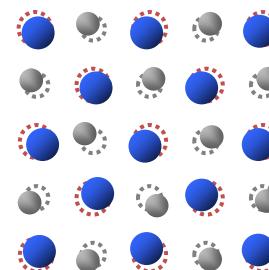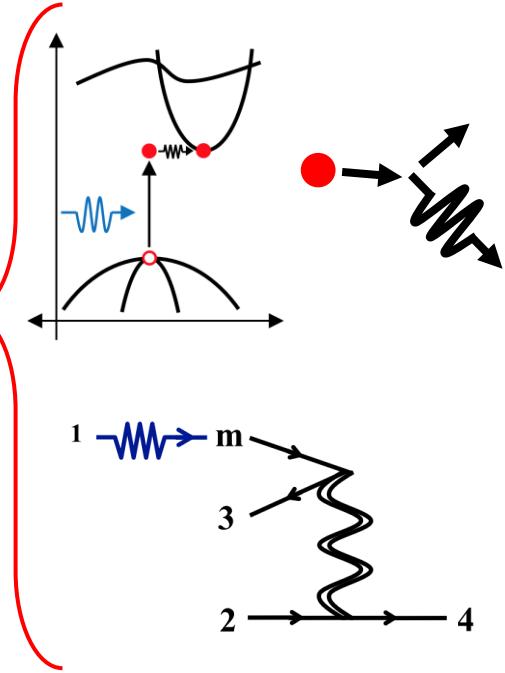
Devices   Materials   Electronic Structure   Quantum Processes

From Macroscopic to Microscopic
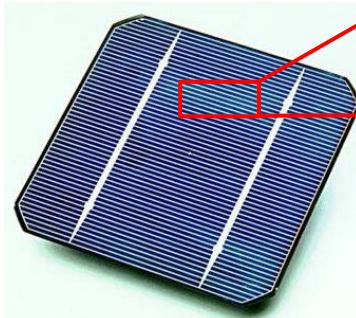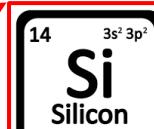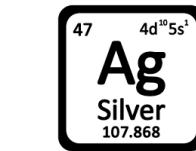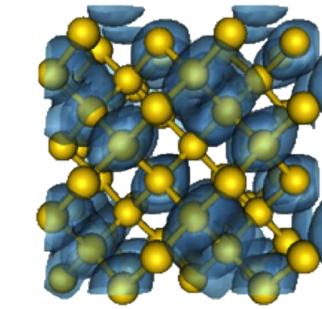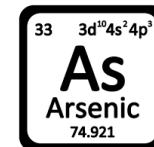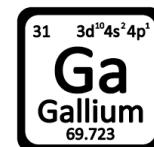
$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v_{KS}(\boldsymbol{r}) \right)\varphi(\boldsymbol{r}) = \varepsilon\varphi(\boldsymbol{r})$$

Semiconductors

Direct and Phonon-assisted Quantum Processes
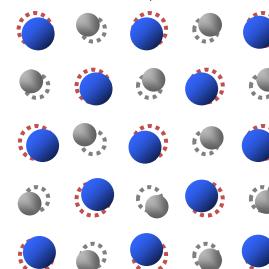
Devices   Materials   Electronic Structure   Quantum Processes
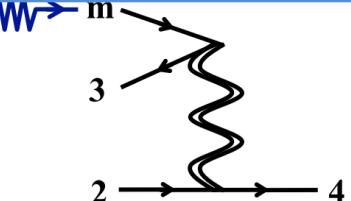
The Benefit of Computation
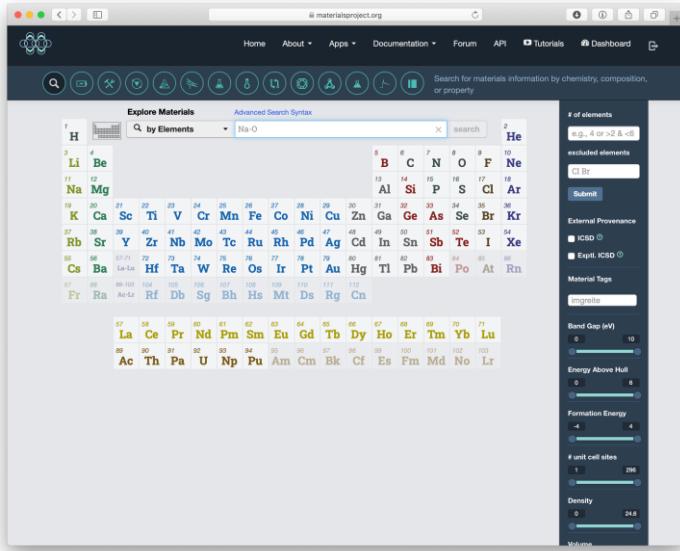

materialsproject.org
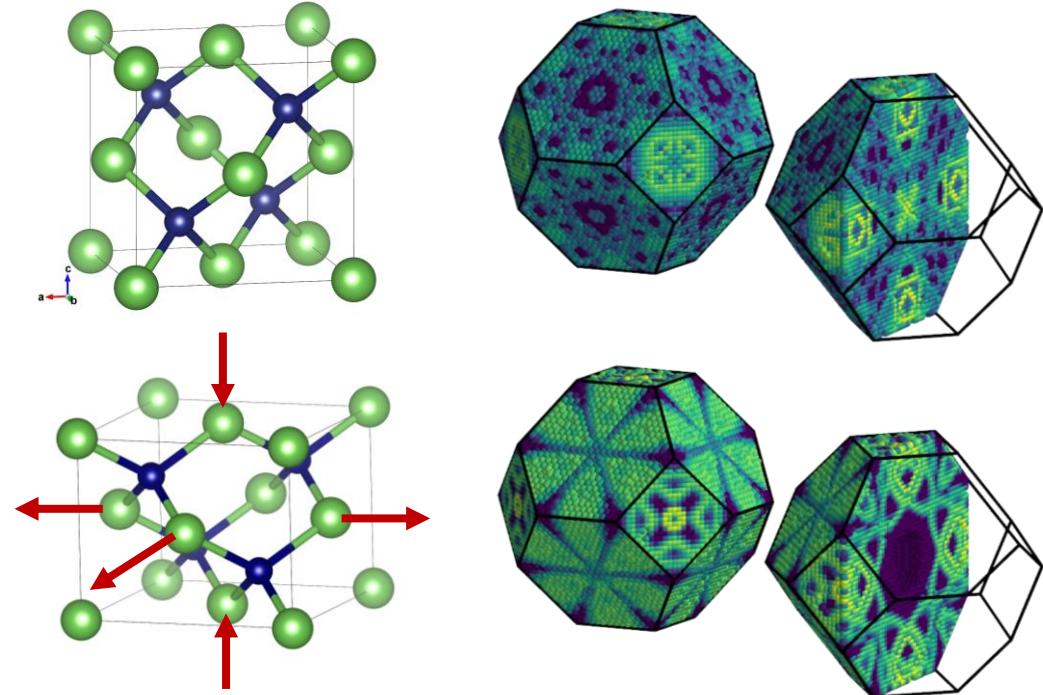
Computational methods can accelerate discovery and improve our understanding of the physics underlying material properties

Computational Toolbox

QUANTUMESPRESSO

BerkeleyGW

EPW
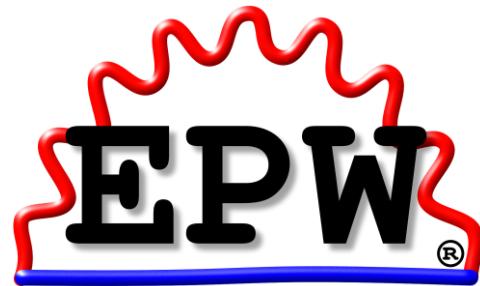
WANNIER90

In-house Auger-Meitner Code*

*name to be determined!

Optical absorption in boron arsenide
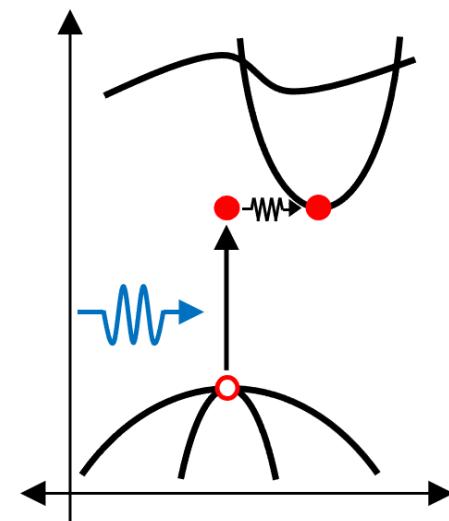
Carrier mobility in boron arsenide and rutile germanium dioxide

Auger-Meitner recombination in silicon

1.87 Å

1.90 Å

Ge   O
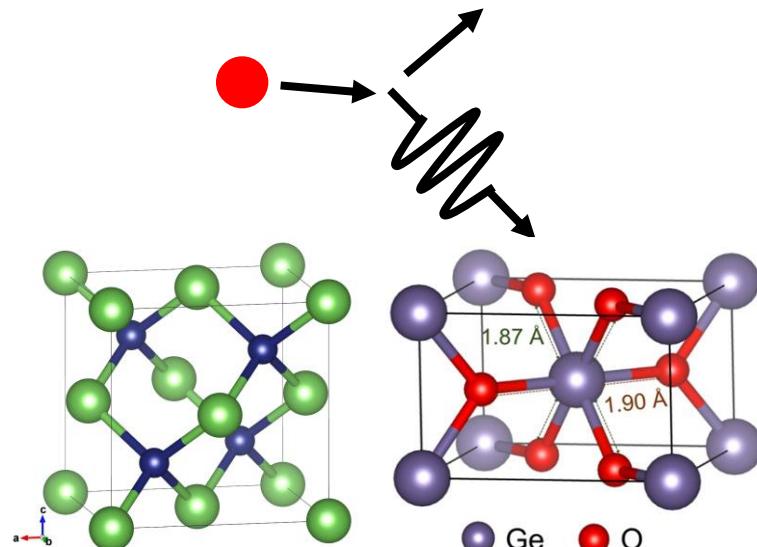
K. Bushick et al., Appl. Phys. Lett. 114, 022101 (2019)

B. Song, K. Chen, K. Bushick et al., Appl. Phys. Lett. 116, 141903 (2020)

K. Bushick et al., npj Comput. Mater. 6, 3 (2020)
K. Bushick et al., Appl. Phys. Lett. 117, 182104 (2020)
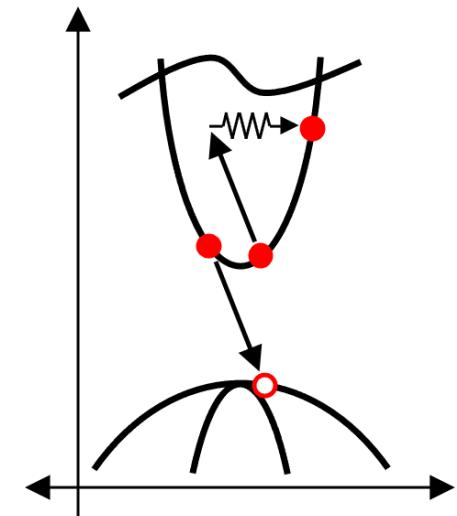
K. Bushick and E. Kioupakis, Phys. Rev. Lett. *Accepted,* (2023)

PHYSICS TODAY

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Home > September 2019 (Volume 72, Issue 9) > Page 10, doi:10.1063/PT.3.4281

A renaming proposal: "The Auger–Meitner effect"

Demetrios Matsakis
(dnmyiasou@yahoo.com) Masterclock, Inc, Washington, DC
Anthea Coster
Massachusetts Institute of Technology Haystack Observatory, Westford
Brenda Laster
Ben-Gurion University, Beer Sheba, Israel
Ruth Sime
Sacramento City College, Sacramento, California
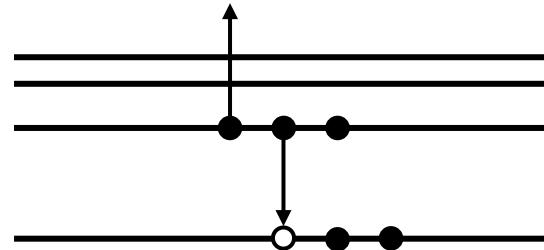
Lise Meitner
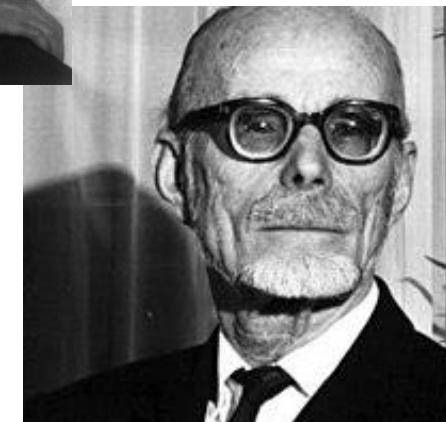
Pierre Auger

Importance of Solar Cells

Planned U.S. utility-scale electric generating capacity additions (2022), gigawatts (GW). Source: U.S. Energy Information Administration, *Preliminary Monthly Electric Generator Inventory*, October 2021
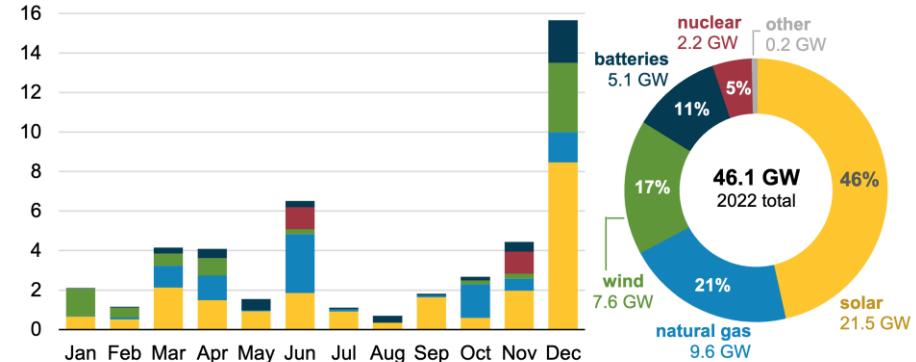
Best Research-Cell Efficiencies (NREL)

$$\tau = \frac{n}{An + Bn^2 + Cn^3}$$

SRH: $R = An$ — Radiative: $R = Bn^2$ — Auger-Meitner: $R = Cn^3$

Data from M.J. Kerr et al. Prog. Photovolt. 11, 97 (2003)

This recombination process involves three carriers near the band edges: either <u>two electrons and a hole</u> (eeh) or <u>two holes and an electron</u> (hhe)

We study two types of Auger-Meitner recombination:
the (a) <u>direct</u> process and (b) <u>phonon-assisted</u> process
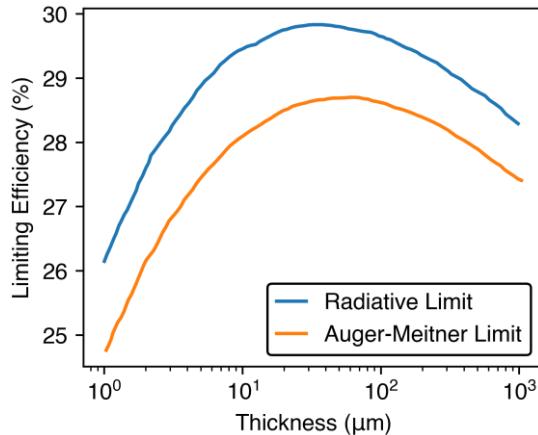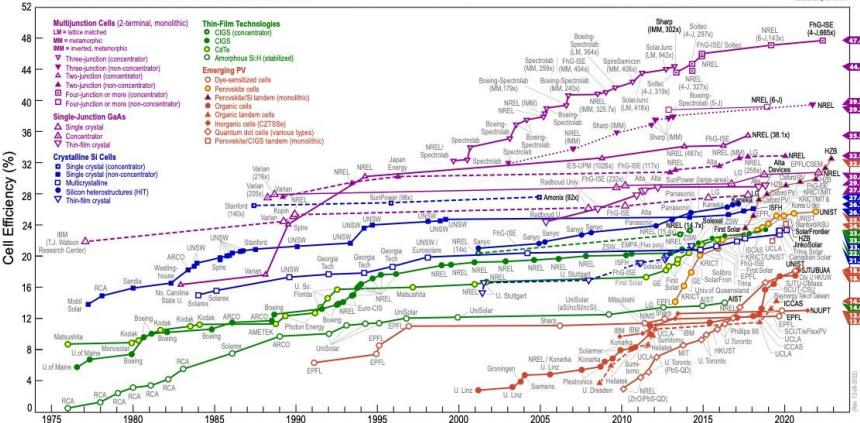
Auger-Meitner Recombination
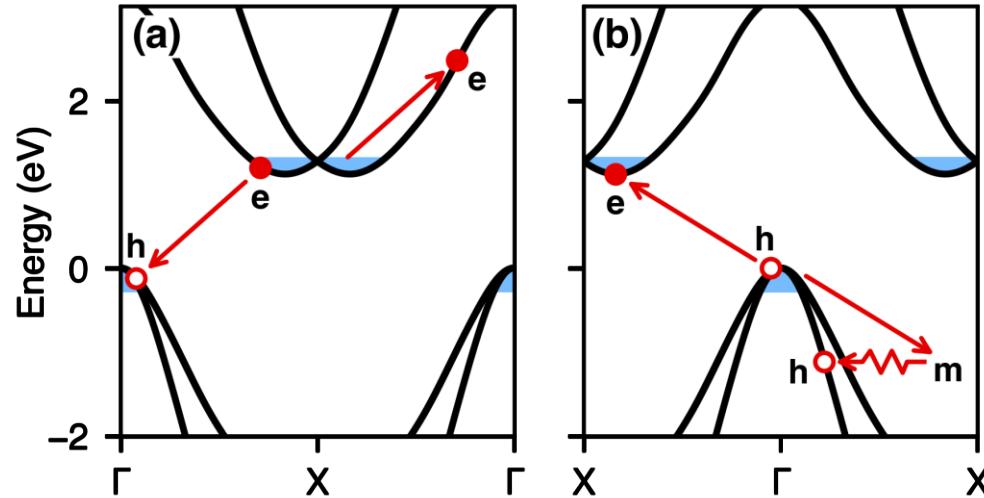
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We study two types of Auger-Meitner recombination:
the (a) <u>direct</u> process and (b) <u>phonon-assisted</u> process

$$\delta(\epsilon_1 + \cdots \mp \hbar\omega_{\nu q})$$

```
verbosity = 1 (valley)
verbosity = 2 (band)
verbosity = 3 (phonon)
verbosity = 4 (k4)
verbosity = 5 (p_mag)
```
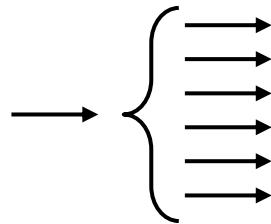
Increased parallelism
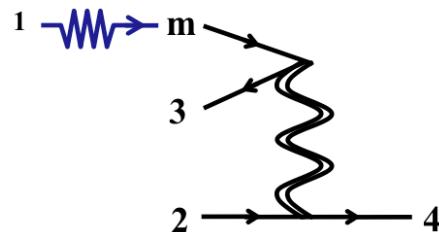
Rewrote and generalized the phonon-assisted code

Added explicit energy conservation constraints

Added different verbose modes for analysis

GNUparallel

Leverage processor parallelism for serial executables

**MPI-IO**

Parallelized IO, binary data
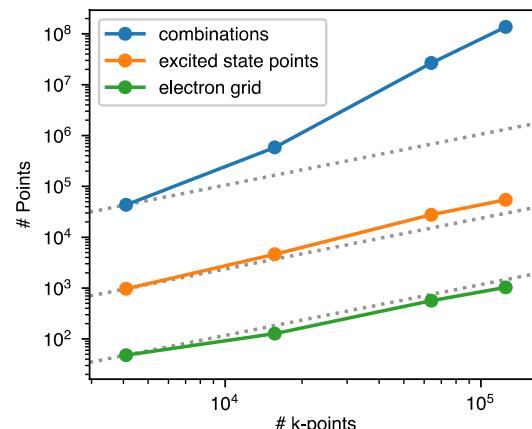
A direct run evaluates:
100,000 wavefunctions (>1 TB)
200,000,000 M_{1234} terms

A phonon-assisted run evaluates:
300,000 wavefunctions (>4 TB)
150,000,000 $\widetilde{M}_{1234;\nu q}$ terms

# AMR vs Carrier Concentration
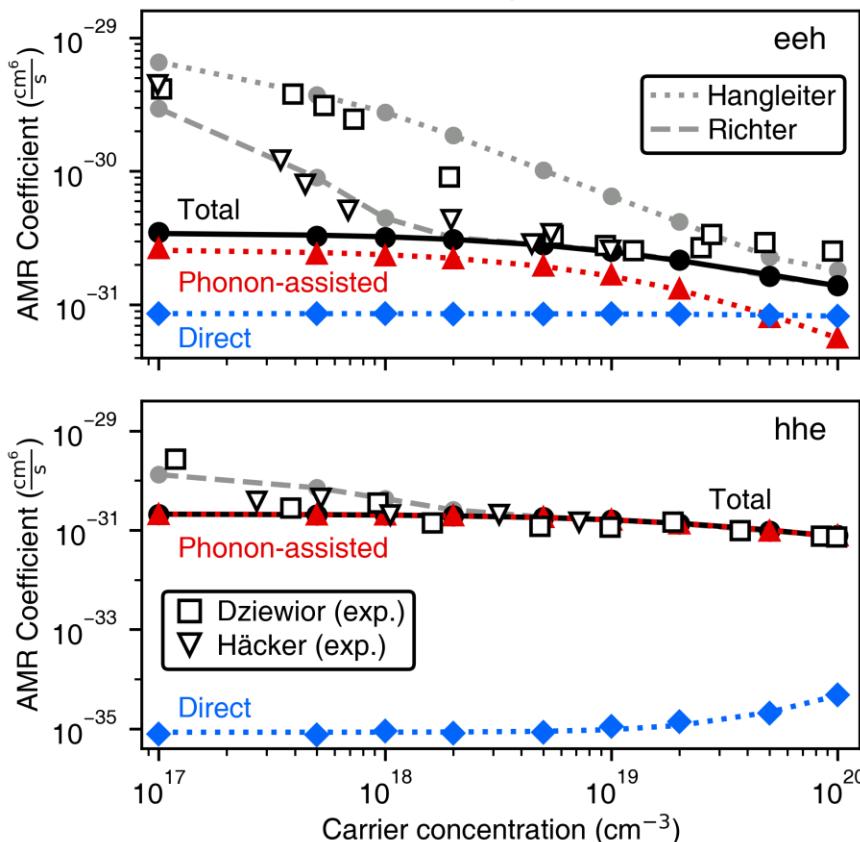
A. Hangleiter and R. Häcker, Phys. Rev. Lett. 65, 215 (1990)
A. Richter, et al., Phys. Rev. B. 86, 165202 (2012)
J. Dziewior and W. Schmid, Appl. Phys. Lett. 31, 346 (1977)
R. Häcker and A. Hangleiter, J. Appl. Phys. 75, 7570 (1994)

Phonon-assisted Auger-Meitner recombination must be considered <u>not only for the hhe process, but also for the eeh process</u>

A. Hangleiter and R. Häcker, Phys. Rev. Lett. 65, 215 (1990)
A. Richter, et al., Phys. Rev. B. 86, 165202 (2012)
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Summary

Tons of Tools

Many Materials

Plenty of Physics

Informative Insights

Societal Significance

Acknowledgements

University of Michigan
- Prof. Emmanouil Kioupakis
- Kioupakis Research Group

MIT
- Prof. Gang Chen
- Prof. Bai Song (now Peking University)
- Dr. Ke Chen

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- Prof. Feliciano Giustino (UT Austin)
- Dr. Hyungjun Lee (now EPFL)

LLNL (practicum)
- Dr. Brandon Wood
- Dr. Tim Hsu
- Dr. James Chapman (now Boston University)
- Dr. Kyoung Kweon

The entire Krell staff!