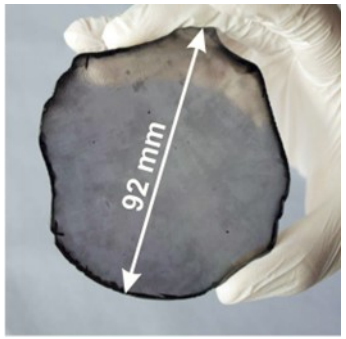
Influence of Deformation Potential Scattering on Impact Ionization in Ultra-Wide Bandgap Materials

Jonah Shoemaker, Reza Vatan, Tathagata Biswas, Arunima Singh, M. Saraniti, Stephen Goodnick

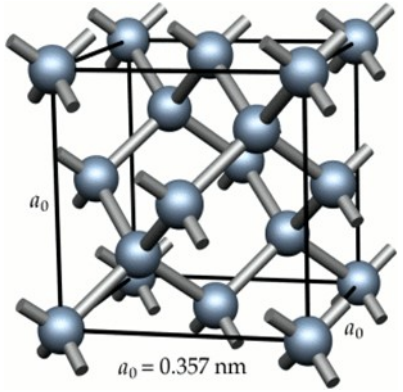
ULTRA Semiconductors



Augsburg Univ.

HexaTech

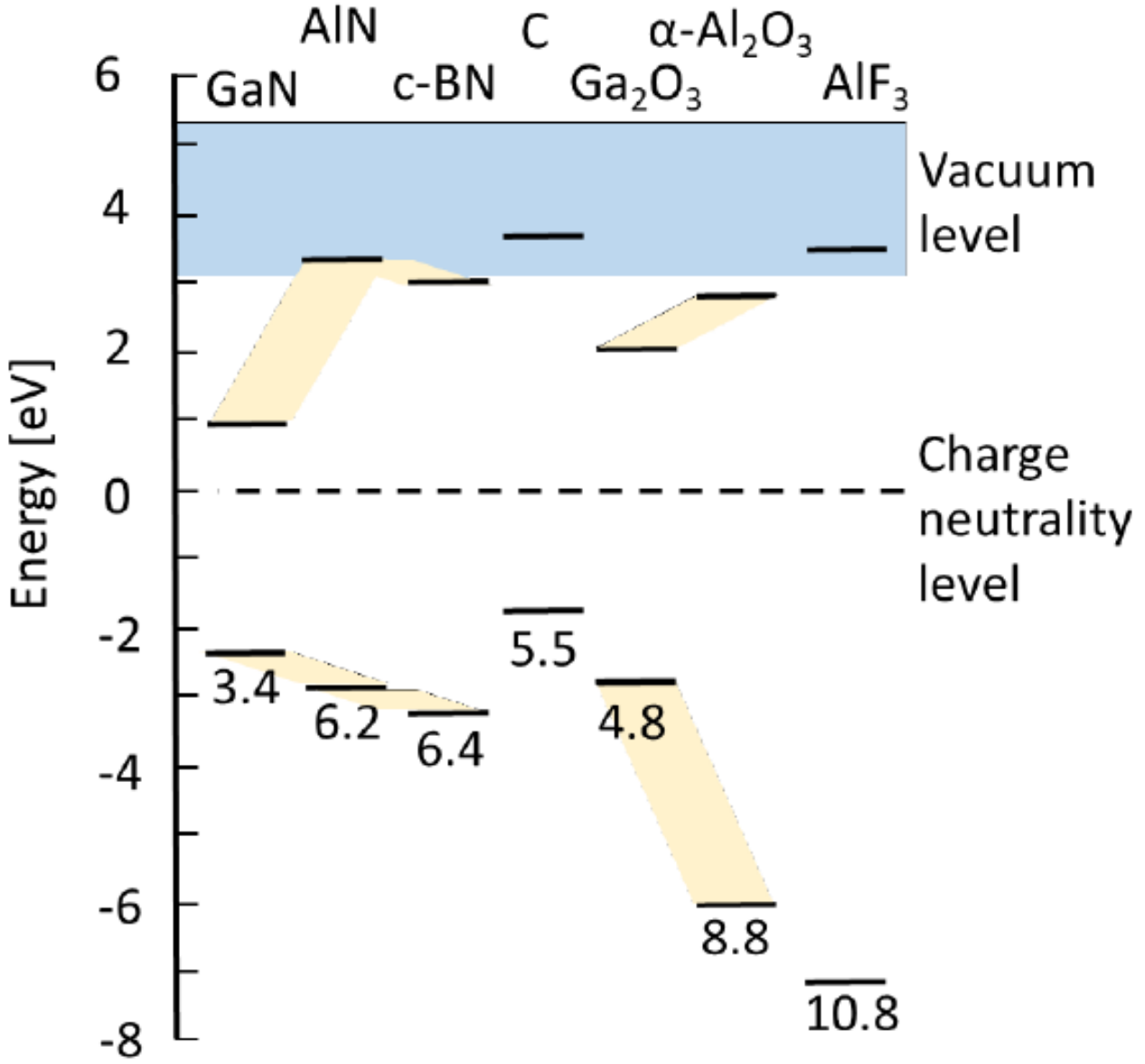
Diamond Cubic



- Eg = 5.5 eV
- sp^3 bonded carbon
- C – 6e
- Diamond Cubic
  a = 3.57 Å

Why ULTRA materials for power electronics: Large bandgap gives high breakdown voltage (limited by avalanche breakdown) and hence high figure of merit:

$$FOM = \frac{V_B^2}{R_{on,sp}}$$

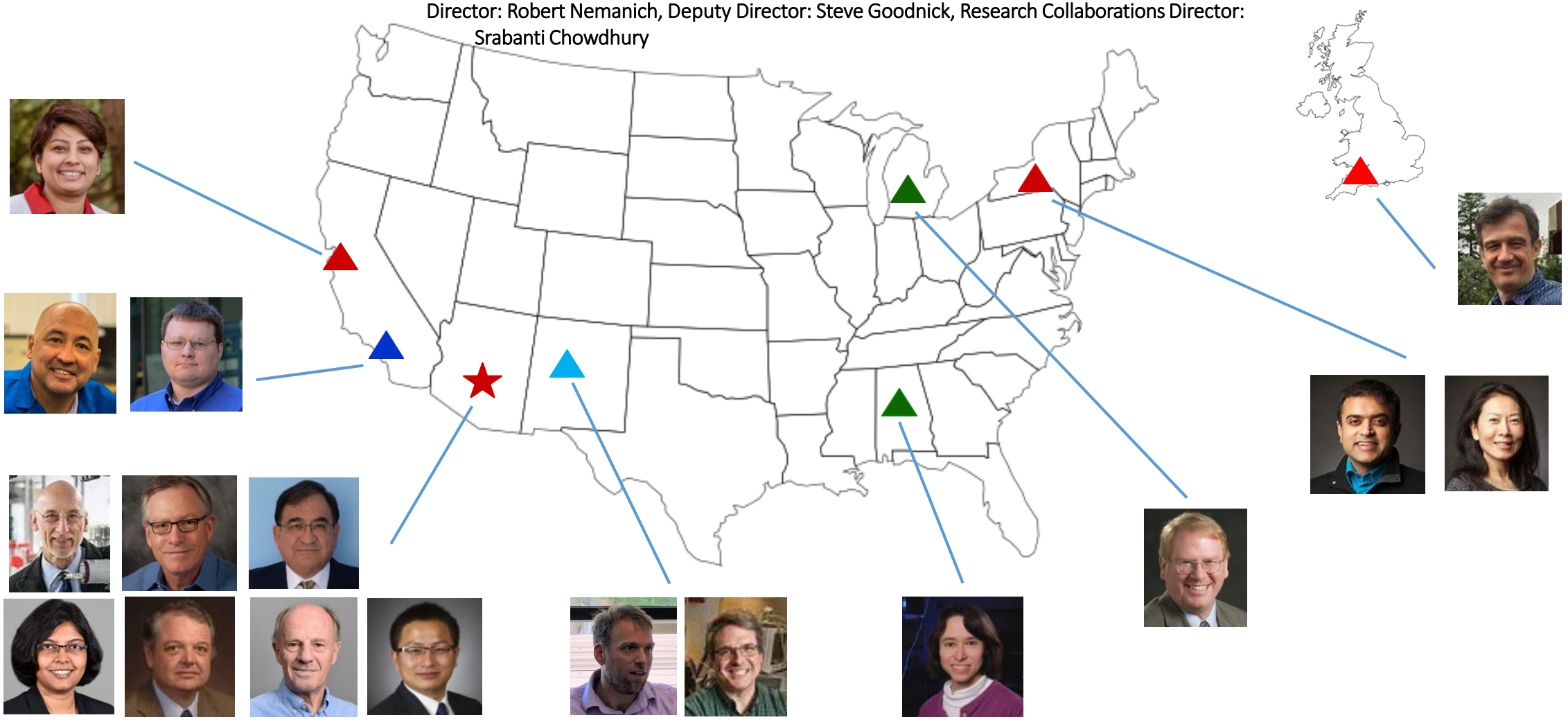


G. L. Doll, J. A. Sell, C. A. Taylor II, and R. Clarke, Phys. Rev. B, **43**, 6816 (1991).

U.S. DEPARTMENT OF ENERGY | Office of Science

Ultra Materials for a Resilient, Smart Electricity Grid (ULTRA) Energy Frontier Research Center

Director: Robert Nemanich, Deputy Director: Steve Goodnick, Research Collaborations Director: Srabanti Chowdhury



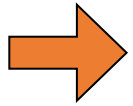
Arizona State University | THE UNIVERSITY OF ALABAMA AT BIRMINGHAM | UC RIVERSIDE | Cornell University | MICHIGAN STATE UNIVERSITY | Sandia National Laboratories | Stanford University | University of BRISTOL

Full Band Cellular Monte Carlo

particle dynamics

Ensemble Monte Carlo (EMC)

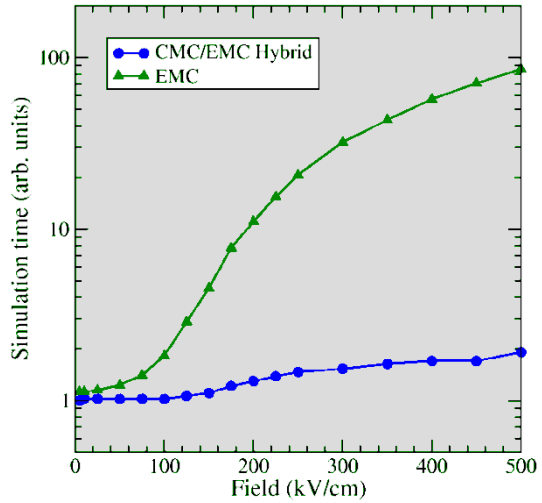
- ✓ computationally slow
- ✓ low memory requirements



choose scattering

new energy

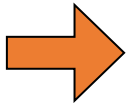
find new k with dispersion relation



vs.

Cellular Monte Carlo (CMC)

- ✓ computationally fast
- ✓ high memory requirements

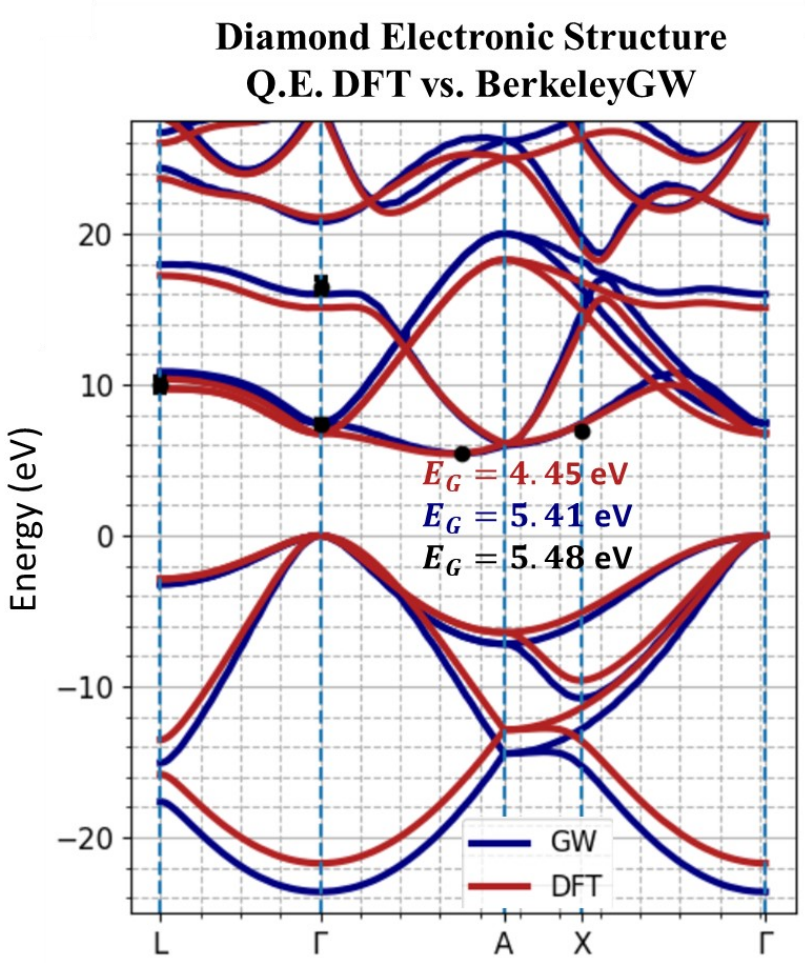


choose new k

M. Saraniti and S.M. Goodnick, *IEEE TED*, 47, 1909 (2000)

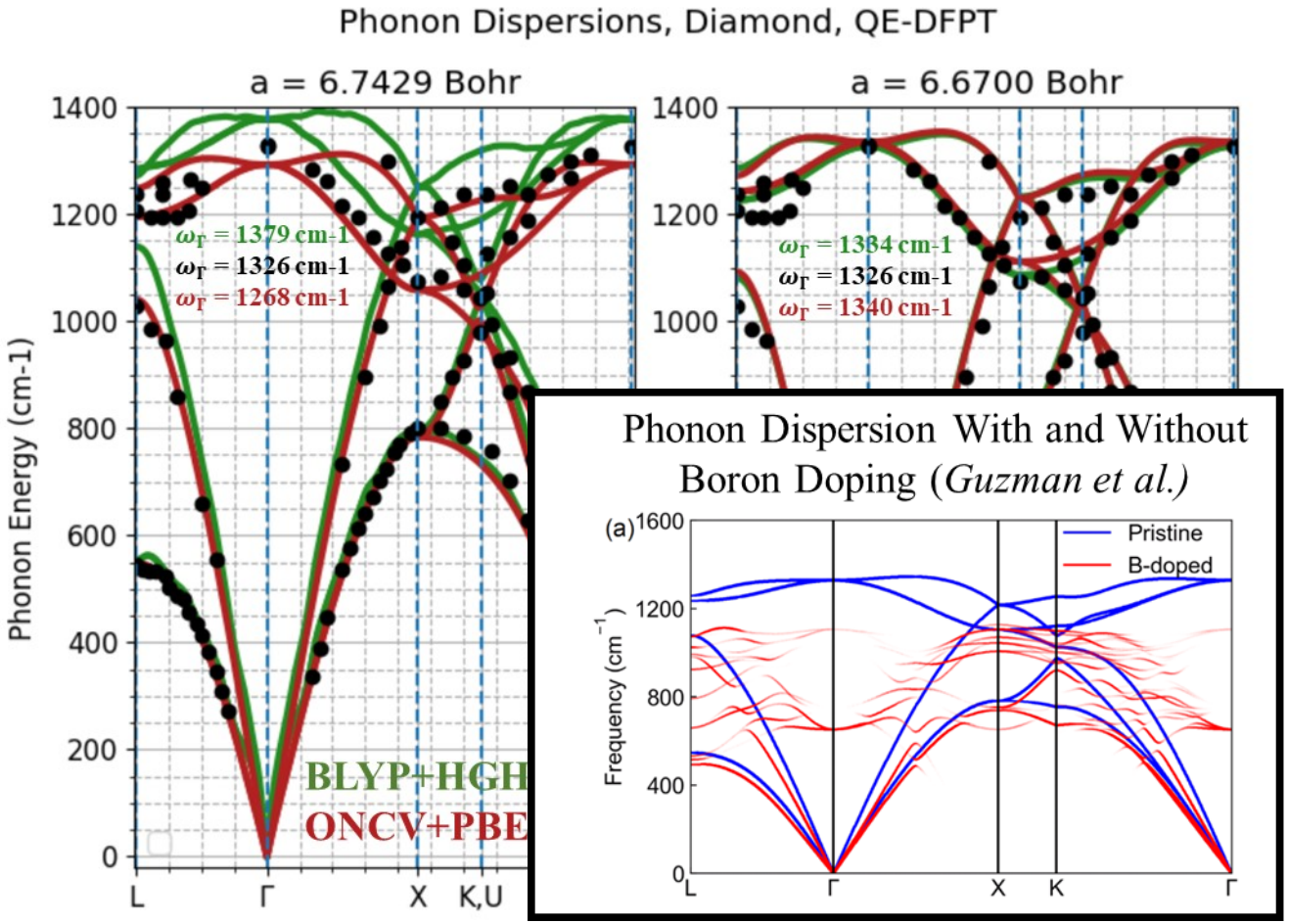
Electronic Structure

- Density Functional Theory (DFT) in Quantum Espresso (QE) is used to calculate the electronic band structure based on the ground-state charge density, computed using pseudopotential inputs.
- BerkeleyGW uses the DFT result from QE as a starting point, and calculates excited states (i.e. conduction band energies) more accurately using Green's functions.
- DFT typically under-estimates band-gaps, while GW produces more accurate estimations.
  - GW band-gap estimations get more accurate with self-consistent iterative solutions.
  - The DFT conduction bands on the right have been shifted upward to match the GW band-gap.



Phonon Dispersion

- Phonon frequencies are computed using Density Functional Perturbation Theory (DFPT) in Quantum Espresso
- The choice of pseudopotential (PP) input file has a large effect on the resulting dispersion with the commonly used lattice constant in diamond
- A relaxed lattice constant (Pavone et al.) converges phonon dispersions from different PP's together in diamond
- Ultra-soft pseudopotentials (not shown) can reproduce the experimental points more accurately, but aren't compatible with GW algorithms



Pavone, P., et al. *Physical Review B* 48.5 (1993): 3156.
Guzman, Erick, et al. *ACS Applied Materials & Interfaces* 14.37 (2022): 42223-42231.

Impact Ionization Scattering Rate

Two approaches to calculating impact ionization transition rate:

1. **Screened Coulomb interaction – 2 particles, internal**
2. Self-energy from GW (Schilfgaarde et al., Usaka et al.)

Impact ionization rate from screened Coulomb interaction:

$$\frac{1}{\tau} = \frac{2\pi}{\hbar}\frac{V^3}{(2\pi)^9}\sum_{n_1\prime n_2 n_2\prime}\iiint dk_{1\prime}dk_2dk_{2\prime}$$
$$\times |M(n_{1\prime},k_{1\prime},n_{2\prime},k_{2\prime};n_1,k_1,n_2,k_2)|^2$$
$$\times \delta\big(E(k_{1\prime})+E(k_{2\prime})-E(k_1)-E(k_2)\big)$$

$$|M|^2 = |M_D|^2 + |M_E|^2 - (M_D^* M_E + M_D M_E^*)/2$$

$$M_D = \sum_{G_1,G_2,G_{1\prime},G_{2\prime}} a^*_{n_{1\prime},k_{1\prime}}(G_{1\prime})\,a^*_{n_{2\prime},k_{2\prime}}(G_{2\prime})$$
$$\times a_{n_1,k_1}(G_1)\,a_{n_2,k_2}(G_2)\,\frac{e^2}{4\pi\epsilon(q_D,\omega_D)q_D^2}$$
$$\times \delta(k_{1\prime}+G_{1\prime}+k_{2\prime}+G_{2\prime}-k_1-G_1-k_2-G_2)$$

Integration across the hot carrier final state $k_{1\prime}$ and cool carrier initial and final states k_2 and $k_{2\prime}$.

Delta function constraints across energy and momentum eliminate one of the three integrals.

Exchange matrix element M_E is found by switching states 1' and 2'.

Sum across all four states' reciprocal lattice vectors requires full knowledge of the band structure and wave-functions. **(only valid for plane wave expansion)**

Watanabe, Tomokatsu, et al. *Journal of applied physics* 95.9 (2004): 4866-4874.

Kamakura, Y., et al. *2016 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*. IEEE, 2016.

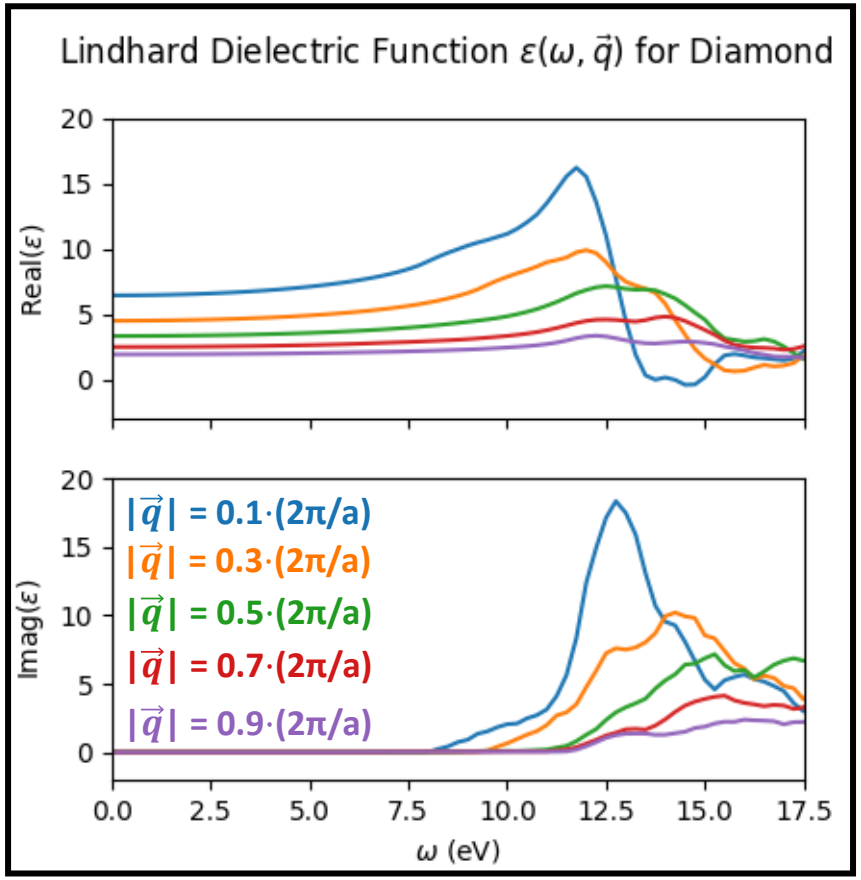
Full-Band Lindhard Dielectric Function

- Full-band and energy-transfer dependence are needed for the dielectric function.
- Static approximation ($\omega = 0$) ceases to be valid when energy transfers on the order of 5-10 eV are taking place to ionize cool carriers across ultra-wide bandgaps.

Full-band-dependent Lindhard dielectric function:

$$\varepsilon_1(\boldsymbol{q},\omega) = \varepsilon_0 + \frac{e^2}{\Omega q^2}\sum_{\Delta\boldsymbol{k},c,v} |\langle \boldsymbol{k}+\boldsymbol{q}, c|\boldsymbol{k}, v\rangle|^2 (\Delta\boldsymbol{k})^3 \times\left\{\frac{1}{E_c(\boldsymbol{k}+\boldsymbol{q})-E_v(\boldsymbol{k})-\hbar\omega}+\frac{1}{E_c(\boldsymbol{k}+\boldsymbol{q})-E_v(\boldsymbol{k})+\hbar\omega}\right\}$$

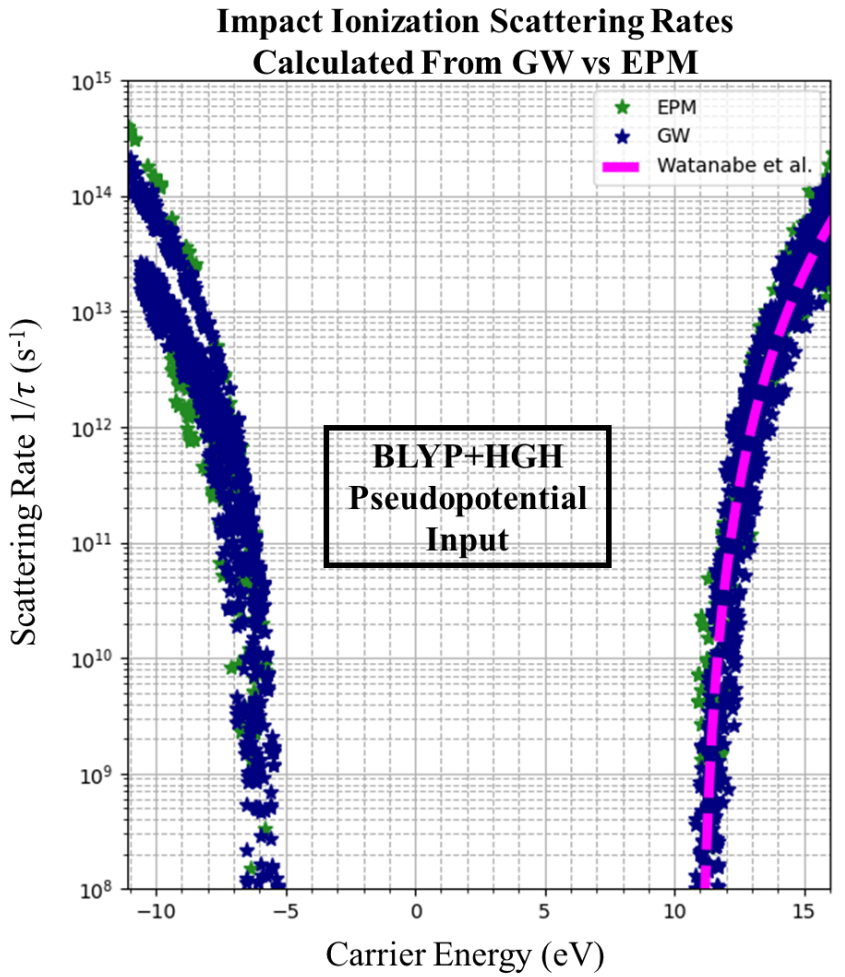
$$\varepsilon_2(\boldsymbol{q},\omega) = \frac{\pi e^2}{\Omega q^2}\sum_{\Delta\boldsymbol{k},c,v} |\langle \boldsymbol{k}+\boldsymbol{q}, c|\boldsymbol{k}, v\rangle|^2 (\Delta\boldsymbol{k})^3 \delta(E_c(\boldsymbol{k}+\boldsymbol{q}) - E_v(\boldsymbol{k}) - \hbar\omega)$$



Dielectric function of diamond along the [100] direction for various values of $|\vec{q}|$

GW-Derived Impact Ionization Scattering Rat

- The CMC code was modified to import BerkeleyGW calculated eigenvalues and wavefunctions
- Using the GW electronic structure as input, the anisotropic impact ionization rate is calculated directly from GW.
- Also possible to directly calculate the impact ionization rate from the self-energy in GW (van Schilfgaarde *Physical Review B 81,* 125201 (2010))



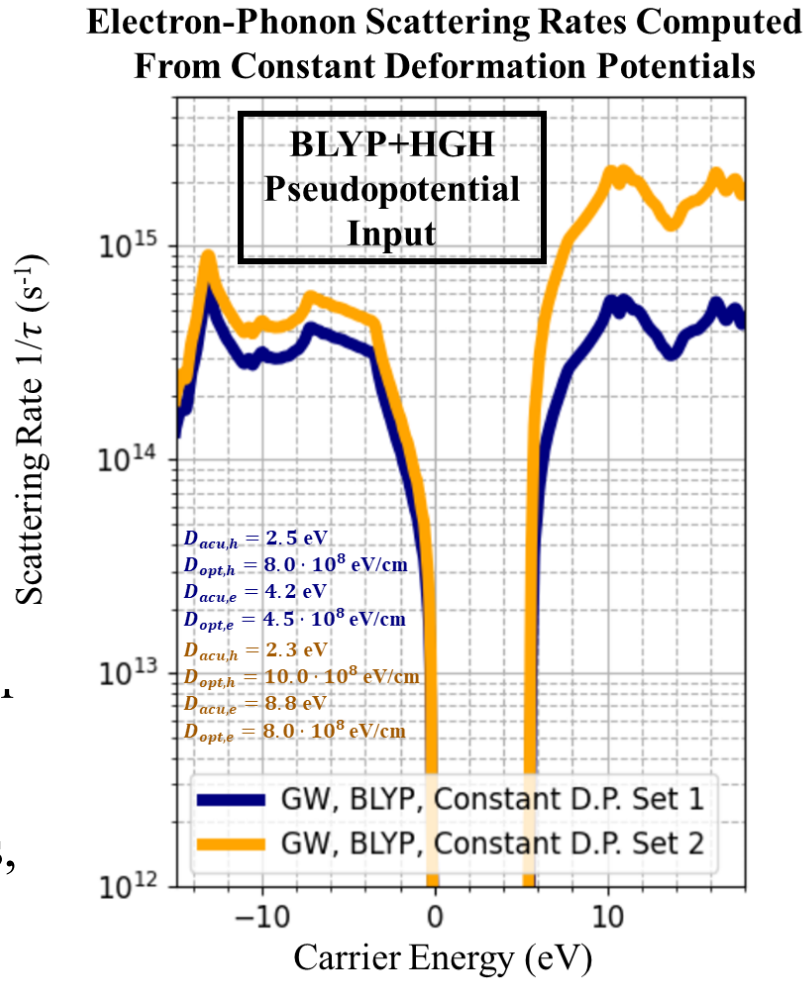
Deformation Potential Scattering

The deformation potential scattering rate from point $\vec{k}$ in band ν to a region $\Omega_{\overrightarrow{k'}}$ centered around the point $\overrightarrow{k'}$ in band ν' for phonon mode η is calculated using Fermi's Golden Rule:

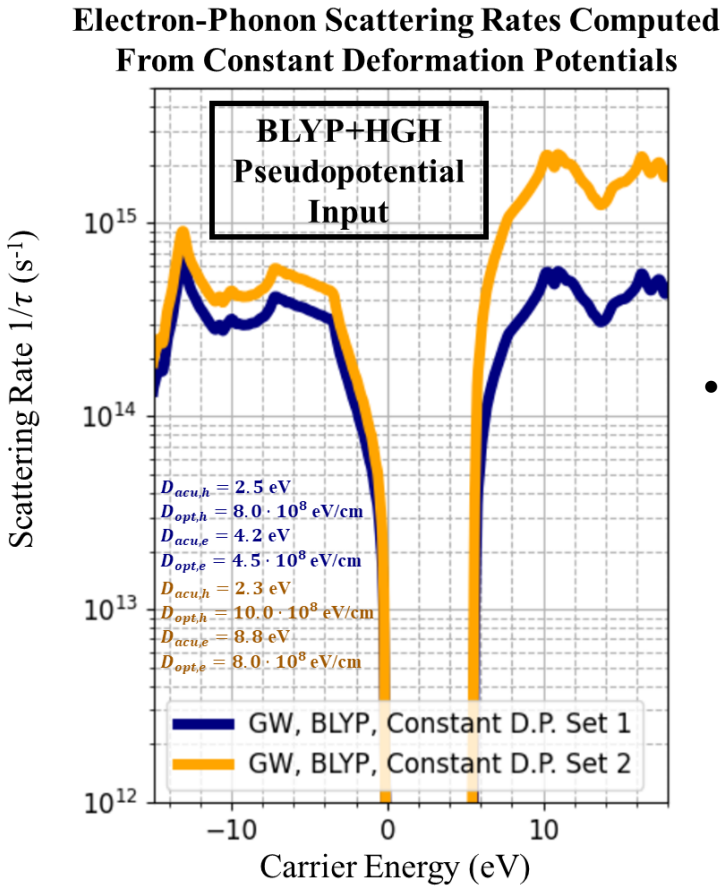
$$\tau^{-1}\left(\vec{k}, \Omega_{\overrightarrow{k'}}, \nu, \nu', \eta\right)$$

$$= \frac{\pi}{\rho\omega_{\eta\vec{q}}}\left|\Delta^{(\eta)}\left(\nu', \vec{k}, \vec{q}, \nu\right)\right|^2 \left|I\left(\nu, \nu', \vec{k}, \overrightarrow{k'}\right)\right|^2 D_{\nu'}\left(\epsilon', \Omega_{\overrightarrow{k'}}\right)\left(N_{\eta\vec{q}} + \frac{1}{2} \mp \frac{1}{2}\right)$$

$\Delta^{(\eta)}(\nu', \vec{k}, \vec{q}, \nu)$ is the deformation potential for phonon mode η between the initial carrier state with wave-vector $\vec{k}$ and band number ν and the final carrier state with $\overrightarrow{k'} = \vec{k} \pm \vec{q}$ and ν'. This has heretofore typically been assumed isotropic and approximated with a constant value for all initial and final states, so that the deformation potential reduces as $\Delta^{(\eta)}\left(\nu', \vec{k}, \vec{q}, \nu\right) \rightarrow \Delta_{const}$.



Impact Ionization Coefficients

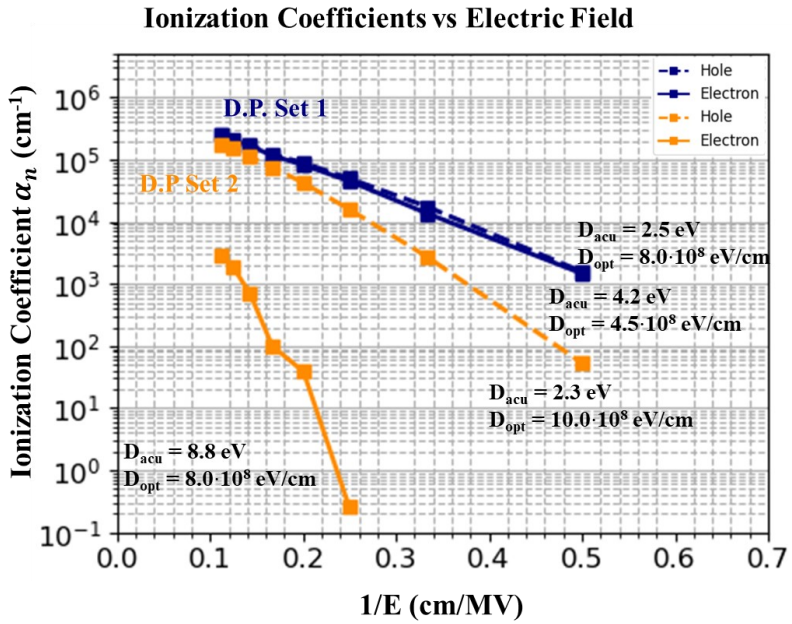


- **Full-Band Monte Carlo simulations with varying E-field strength along the [100] direction**
- **Impact ionization coefficients are calculated for each E-field using**

$$\alpha_i(E) = \frac{1}{N\bar{v}_i(E)} \frac{dn_i(E)}{dt}$$

- **The results are fitted to Chynoweth's law:**

$$\alpha_{n,p} = A_{n,p} exp\left(-\frac{B_{n,p}}{|E|}\right)$$



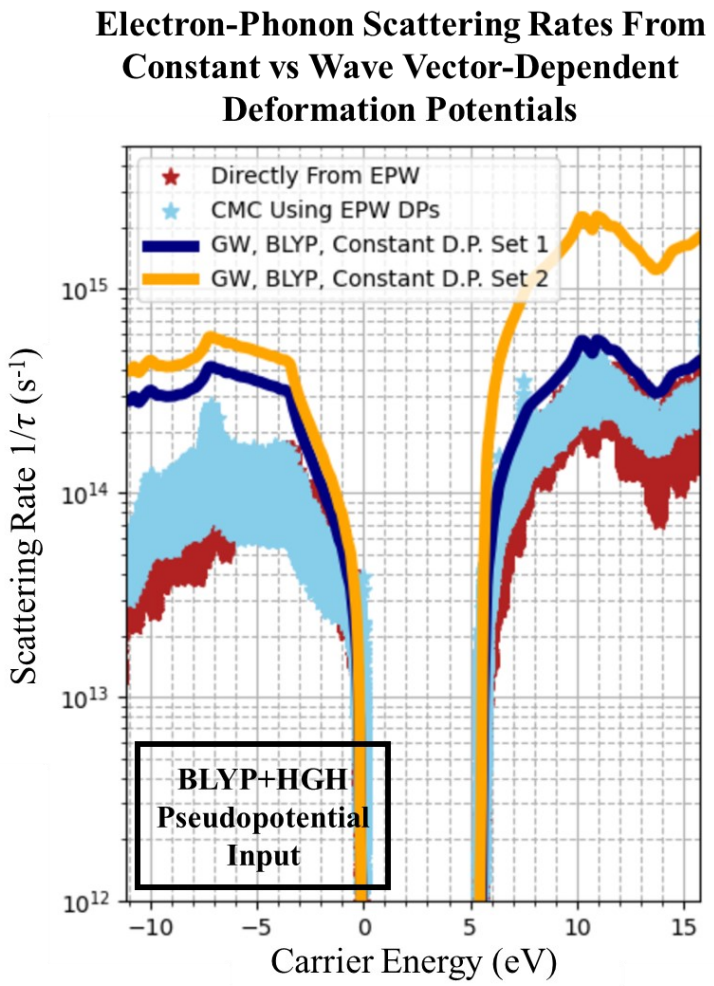
- Large differences between the deformation potentials leads to large discrepancies between ionization coefficient results.
- This motivated us to study EPW (**E**lectron-**P**honon with **W**annier) and first-principles calculations of deformation potentials.

Ab Initio Electron-Phonon Interactions

- The deformation potentials can be obtained from the electron-phonon interaction matrix elements, which are calculated *ab initio* using the EPW (Electron-Phonon using Wannier functions) code suite in Quantum Espresso using

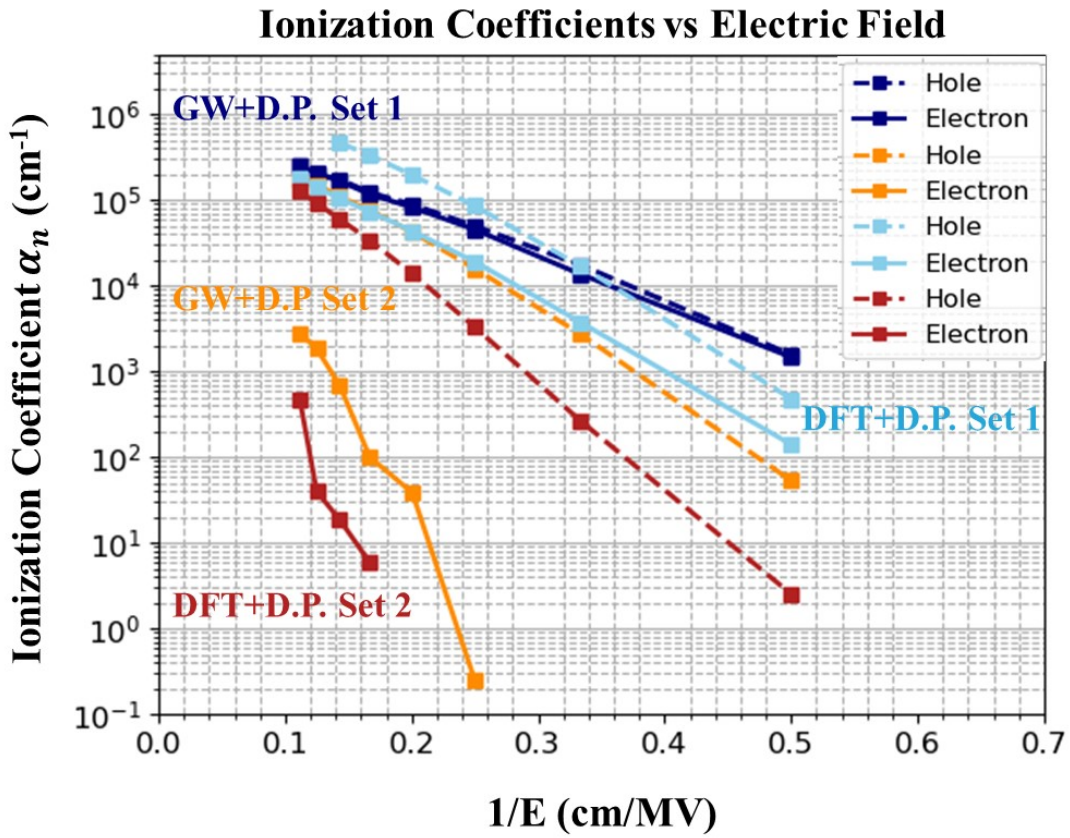
$$g_{\vec{q}\nu}(\vec{k},\nu,\nu') = \left(\frac{\hbar}{2m_0\omega_{\vec{q}\eta}}\right)^{1/2} \left\langle \psi_{\nu,\vec{k}} \left| \frac{dV_{SCF}}{d\hat{u}_{\vec{q}\eta}} \cdot \hat{\epsilon}_{\vec{q}\eta} \right| \psi_{\nu',\vec{k}+\vec{q}} \right\rangle$$

- After extracting the deformation potentials for each $\vec{k}$ to $\vec{k'}$ transition from the EPW code output, we can import the deformation potentials into our CMC code to calculate the deformation potential scattering rates.



Ionization Coefficients in Diamond

- The deformation scattering transition rates obtained from EPW are used with the *ab initio* impact ionization transition rates in bulk diamond full-band Cellular Monte Carlo simulations with varying electric field strengths to obtain the field-dependent ionization rates.
- As observed on the right, importing the *ab initio* deformation potentials from EPW increases the measured ionization rate for both electrons and holes.
- Ionization rates obtained from DFT electronic structure are significantly different from the GW rates, demonstrating that finer band structure features have a notable effect.



Conclusion

- Simulated ionization coefficients are highly dependent on the choice of deformation potential inputs.
- Deformation potentials from *ab initio* methods (EPW) increase the resulting ionization coefficients.
- The choices of electronic and phonon band structure inputs are also important.
- This methodology will be extended to other UWBG materials, including cubic BN and AlN alloys (AlGaN, BAlN).

Velocity Field