Modeling **electronic final states** in **liquid xenon** for light dark matter detection

Theresa M. Backes

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In collaboration with: Andres Tellez Mora, Riccardo Catena, Nicola Spaldin

CHALMERS
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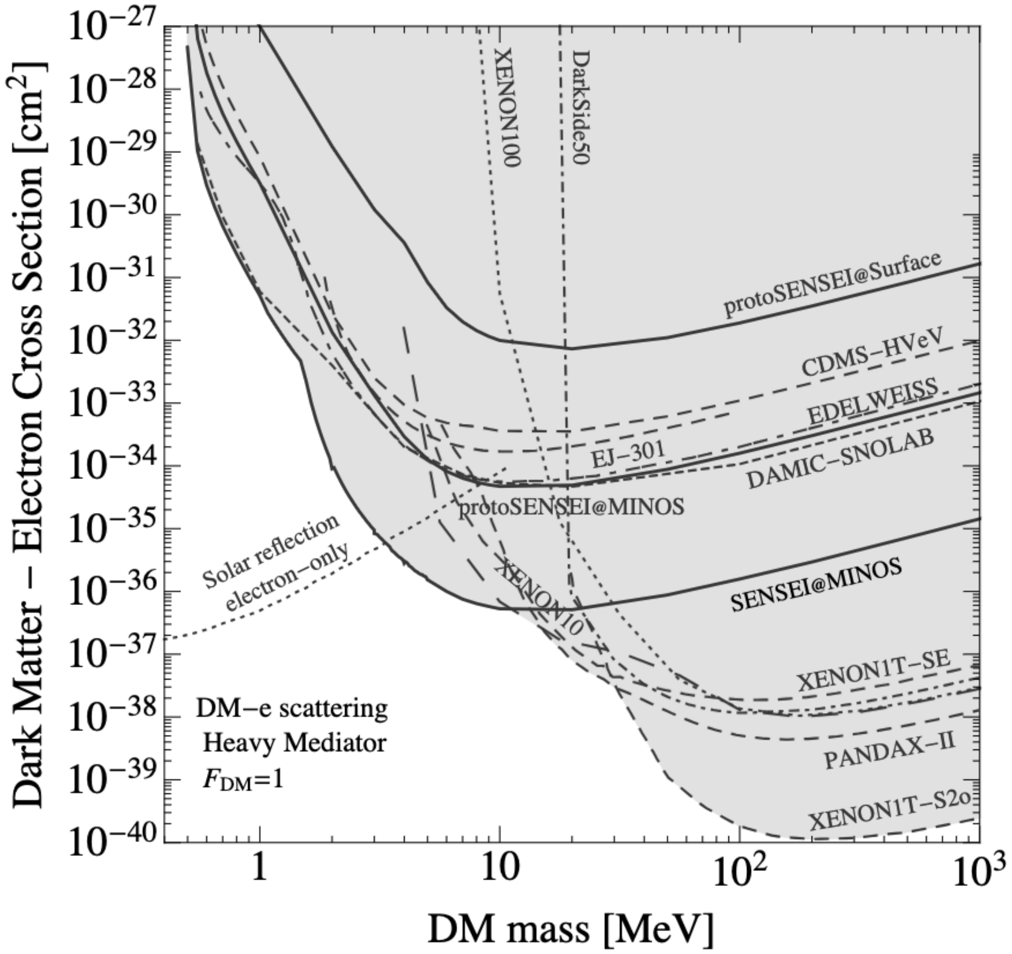
Searching sub-GeV DM with liquid Xenon



Snowmass2021; arXiv:2203.08297

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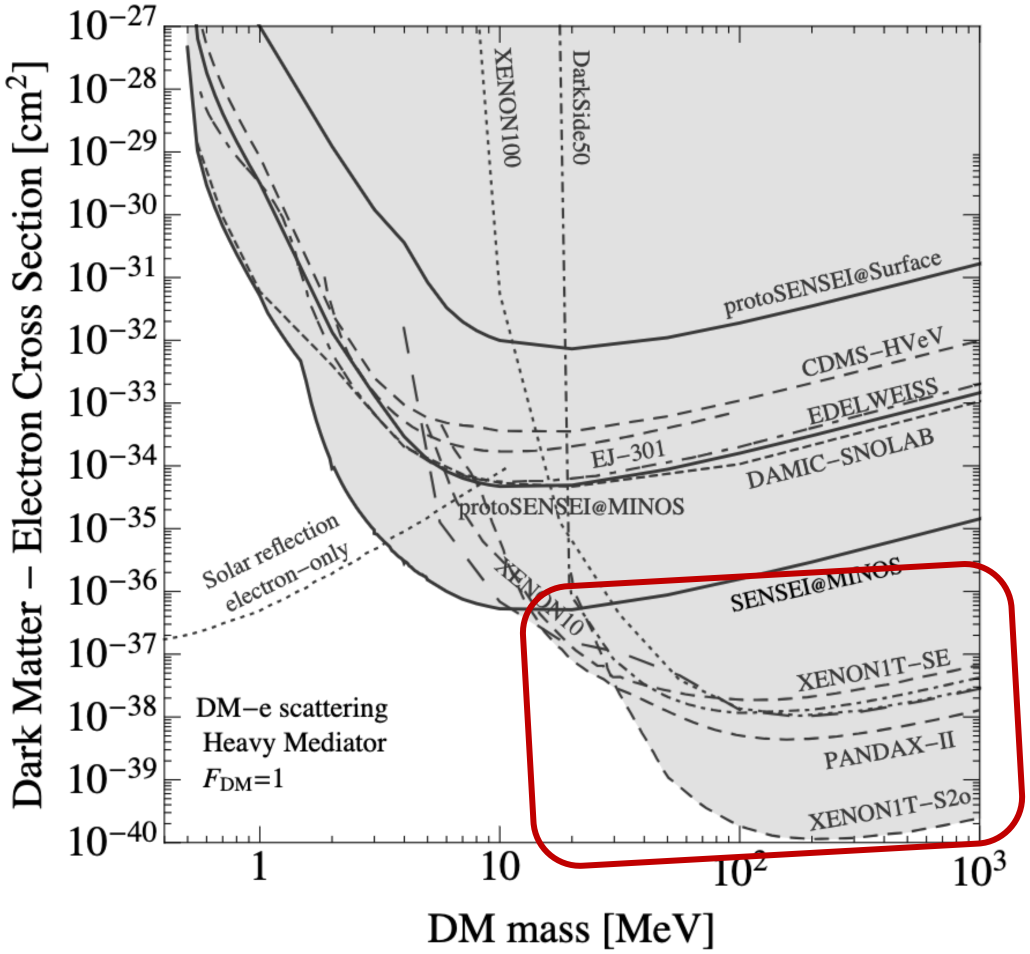

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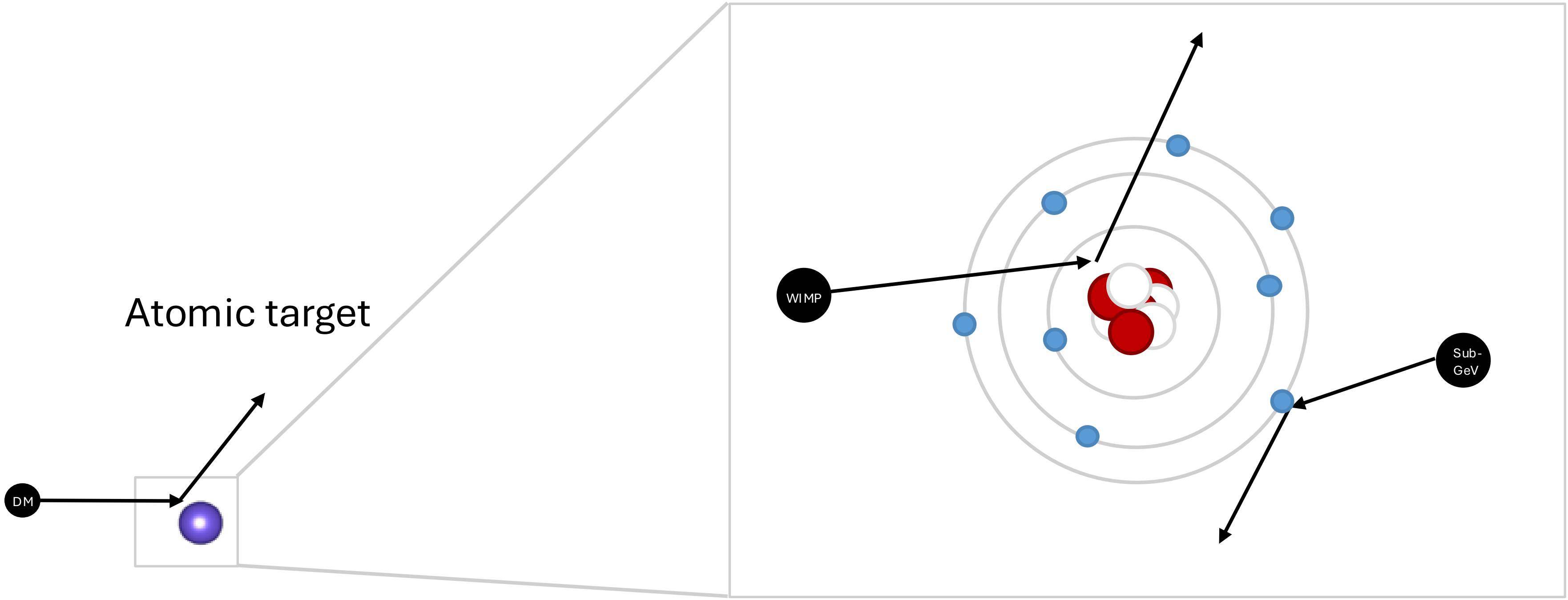
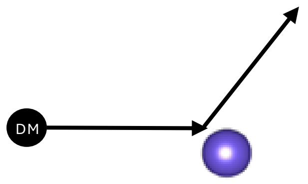
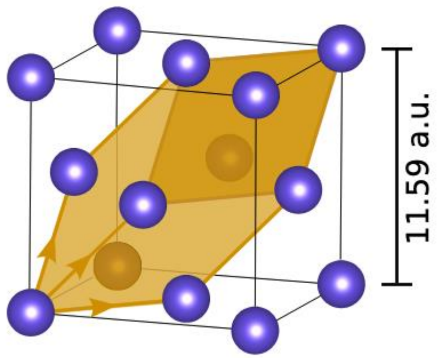


Searching sub-GeV DM with liquid Xenon

Crystal target

Atomic target





Catena et al.; doi:10.21468/SciPostPhys.19.3.064

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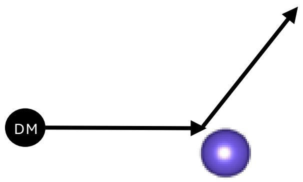

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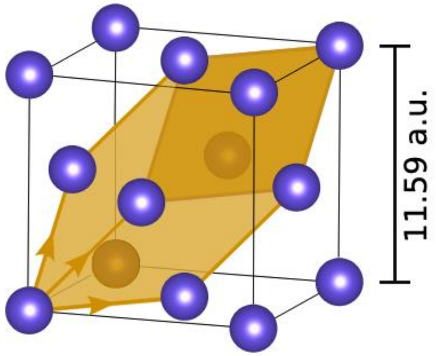
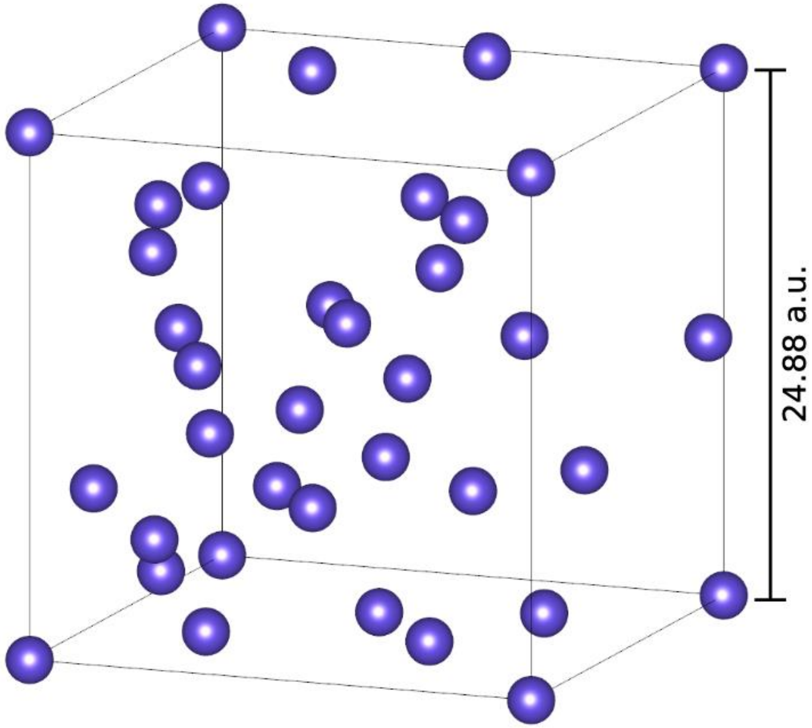


Liquid target



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Electronic states in EXCEED-DM

Calculates DM-electron interaction rates based on the electronic configuration of the target

T. Trickle; doi:10.1103/PhysRevD.107.035035
S. M. Griffin, et al.; doi:10.1103/PhysRevD.104.095015

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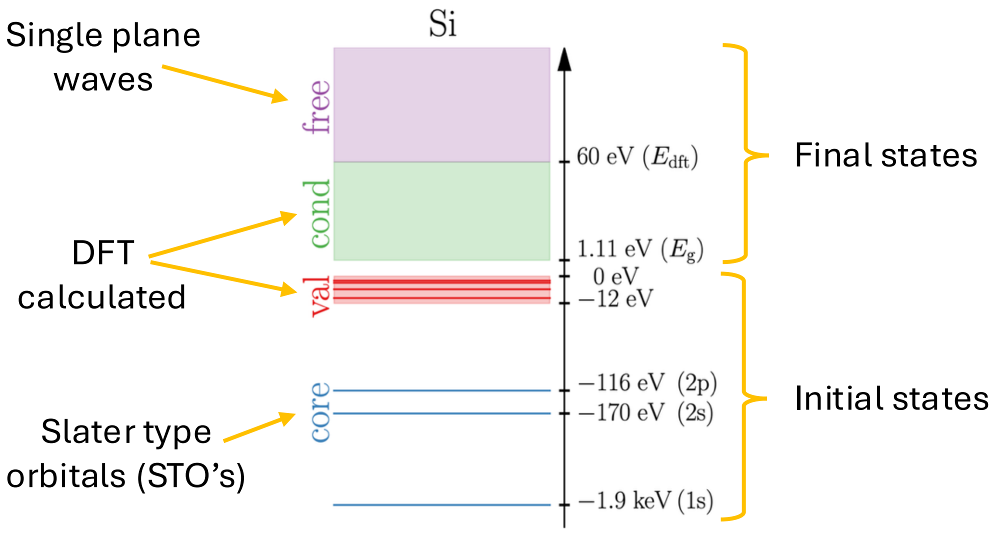

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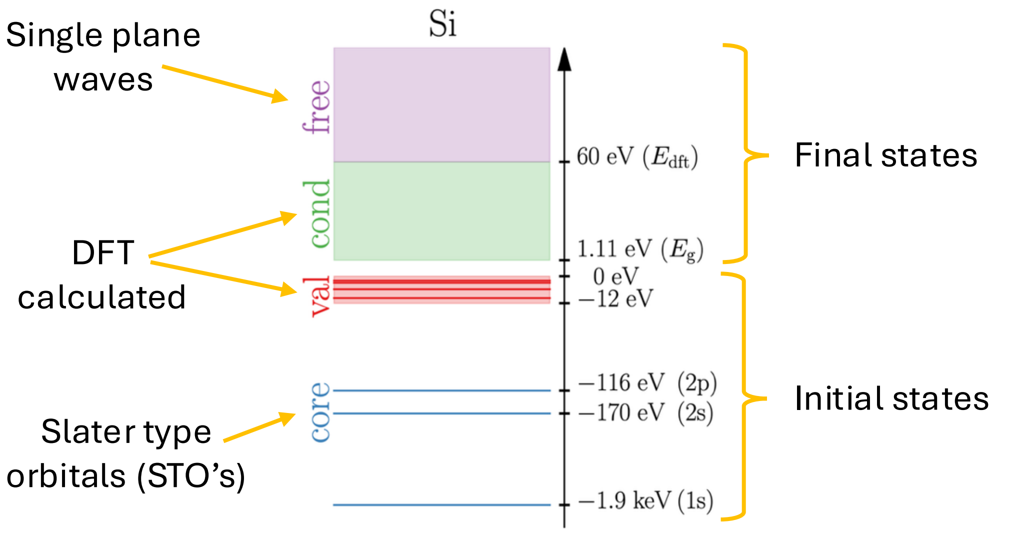


Absorption in **atomic targets**:
G. Krnjaic, T. Trickle; doi:10.1103/PhysRevD.108.015024

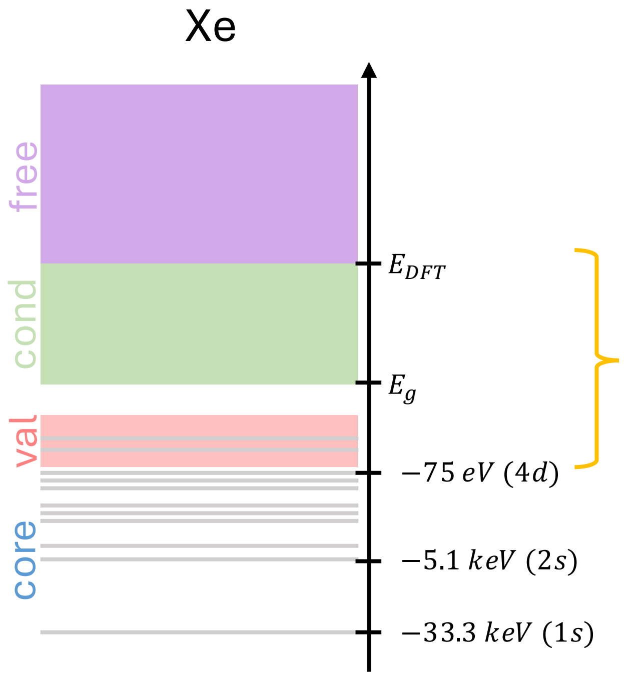
Coulomb states

↑

Core states (STO's)

Isolated Atoms

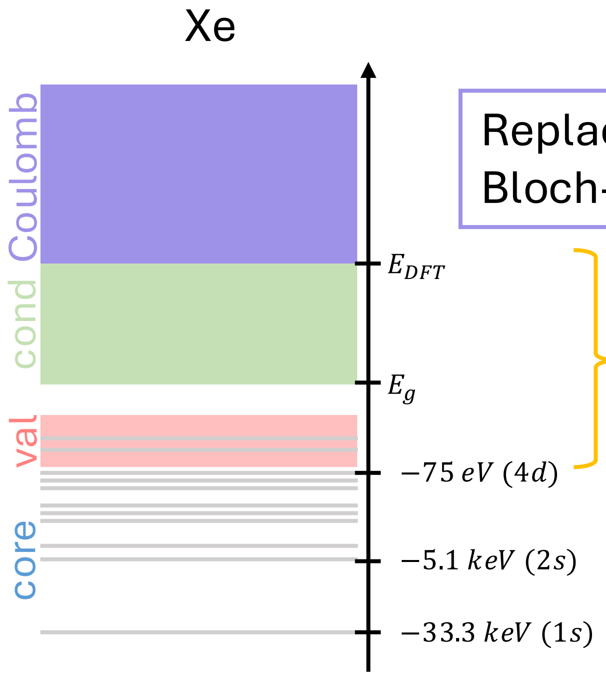
Electronic states of Xenon



DFT + All-electron reconstruction

Ask Andres Tellez Mora

Electronic states of Xenon



Replace single plane waves by Bloch-Coulomb states

DFT + All-electron reconstruction

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New Coulomb states

Positive energy solutions of the Schrödinger equation for isolated atoms:

$$\Psi_{p_f lm}(\mathbf{x}) = \underbrace{R_{\eta l}(x, p_f)}_{\text{Unbound hydrogen-like orbitals}} Y_l^m(\Omega_{\mathbf{x}})$$

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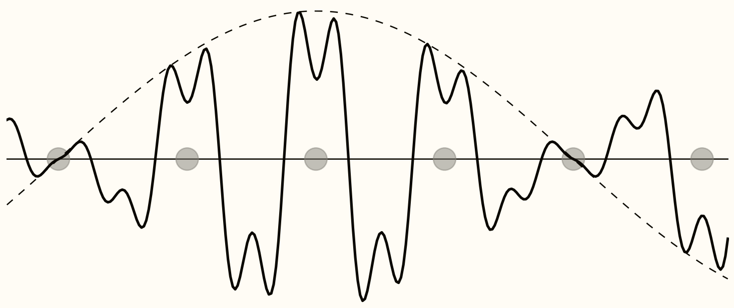
Make it Bloch electrons → We want to describe ionization in a condensed matter system



Bloch wave function:

$$\psi_\mathbf{k}(\mathbf{x}) = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{x}} u_\mathbf{k}(\mathbf{x})$$

Periodic with the lattice

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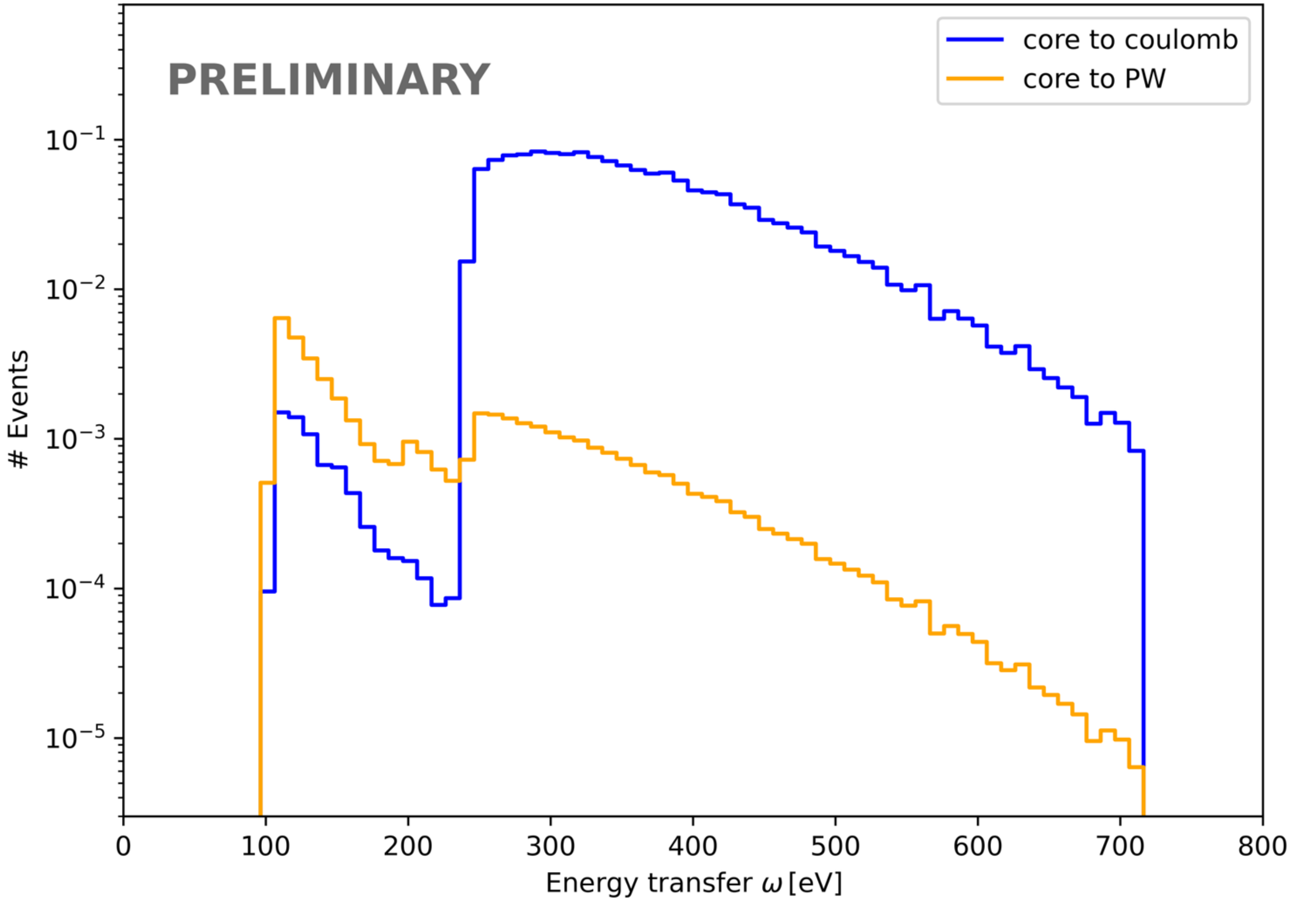
Make it Bloch electrons → We want to describe ionization in a condensed matter system

$$\Psi_{\mathbf{p}_f}(\mathbf{x}) = \frac{1}{\sqrt{V}} e^{i\mathbf{p}_f \cdot \mathbf{x}} \sum_{\mathbf{r}} \sum_{\mathbf{x}_{eq}} e^{i\mathbf{p}_f \cdot (\mathbf{x} - \mathbf{r} - \mathbf{x}_{eq})} \cdot 4\pi \sum_{l} \sum_{m} i^l e^{i\sigma_l} R_{\eta l}(x - r - x_{eq}, p_f) \cdot Y_l^m(\Omega_{\mathbf{x}-\mathbf{r}-\mathbf{x}_{eq}}) Y_l^m(\Omega_{\mathbf{p}_f})$$

Inspired by ARPES (Angle Resolved Photo Emission Spectroscopy)
C. Kern et al.; doi:10.1103/PhysRevResearch.5.033075

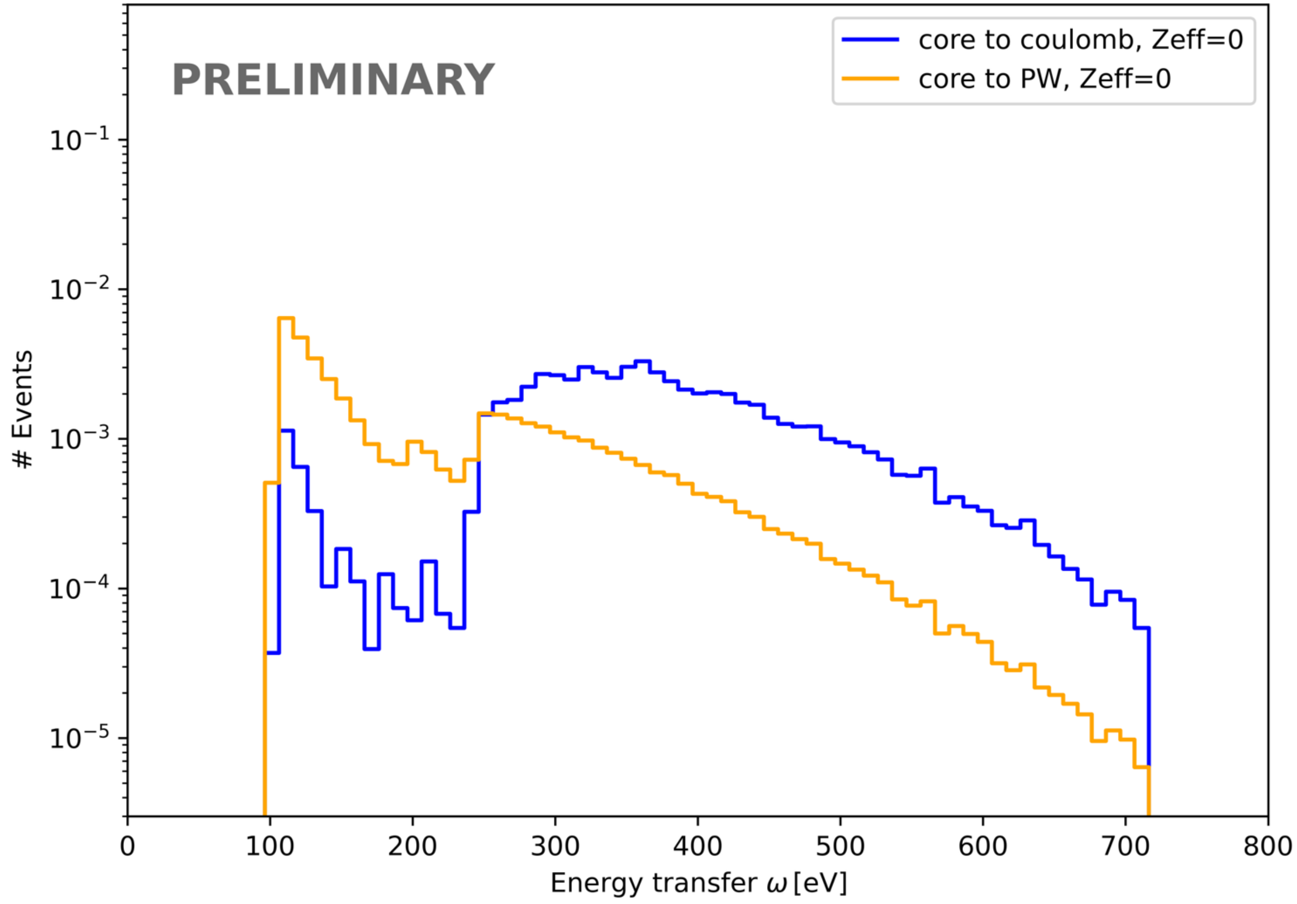
First test for crystalline Xenon



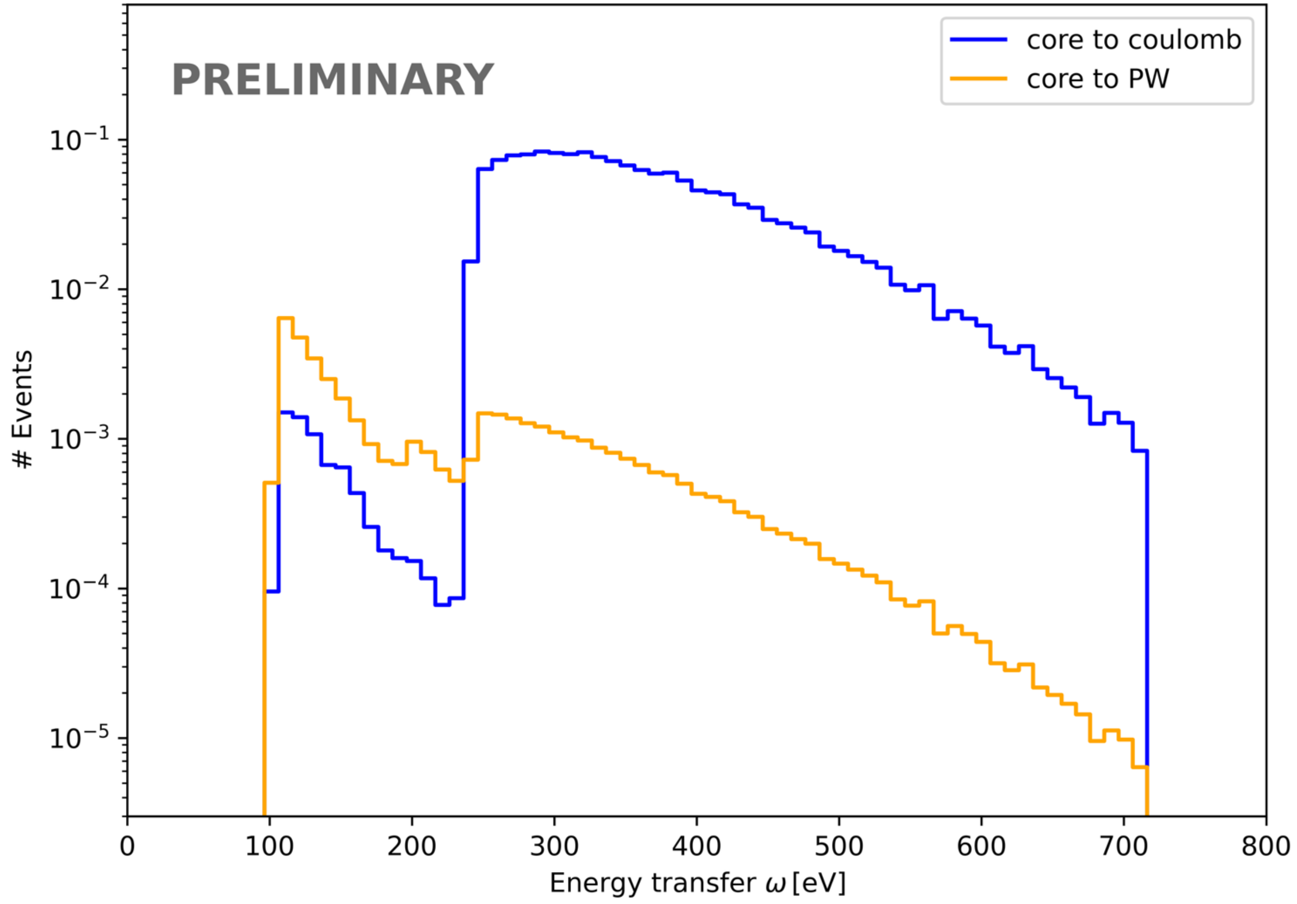
Sanity check

$$\Psi_{\mathbf{p}_f}(\mathbf{x}) = \frac{1}{\sqrt{V}} e^{i\mathbf{p}_f\cdot\mathbf{x}} \sum_{\mathbf{r}} \sum_{\mathbf{x}_{eq}} e^{i\mathbf{p}_f\cdot(\mathbf{x}-\mathbf{r}-\mathbf{x}_{eq})}$$
$$\cdot 4\pi \sum_l \sum_m i^l e^{i\sigma_l} R_{\eta l}(x - r - x_{eq}, p_f)$$
$$\cdot Y_l^m(\Omega_{\mathbf{x}-\mathbf{r}-\mathbf{x}_{eq}}) Y_l^m(\Omega_{\mathbf{p}_f})$$

For $\eta = \dfrac{Z_{eff}}{a_0\, p_f} \to 0$ the Coulomb states become plane waves



Potential problem: sampling of the unit cell



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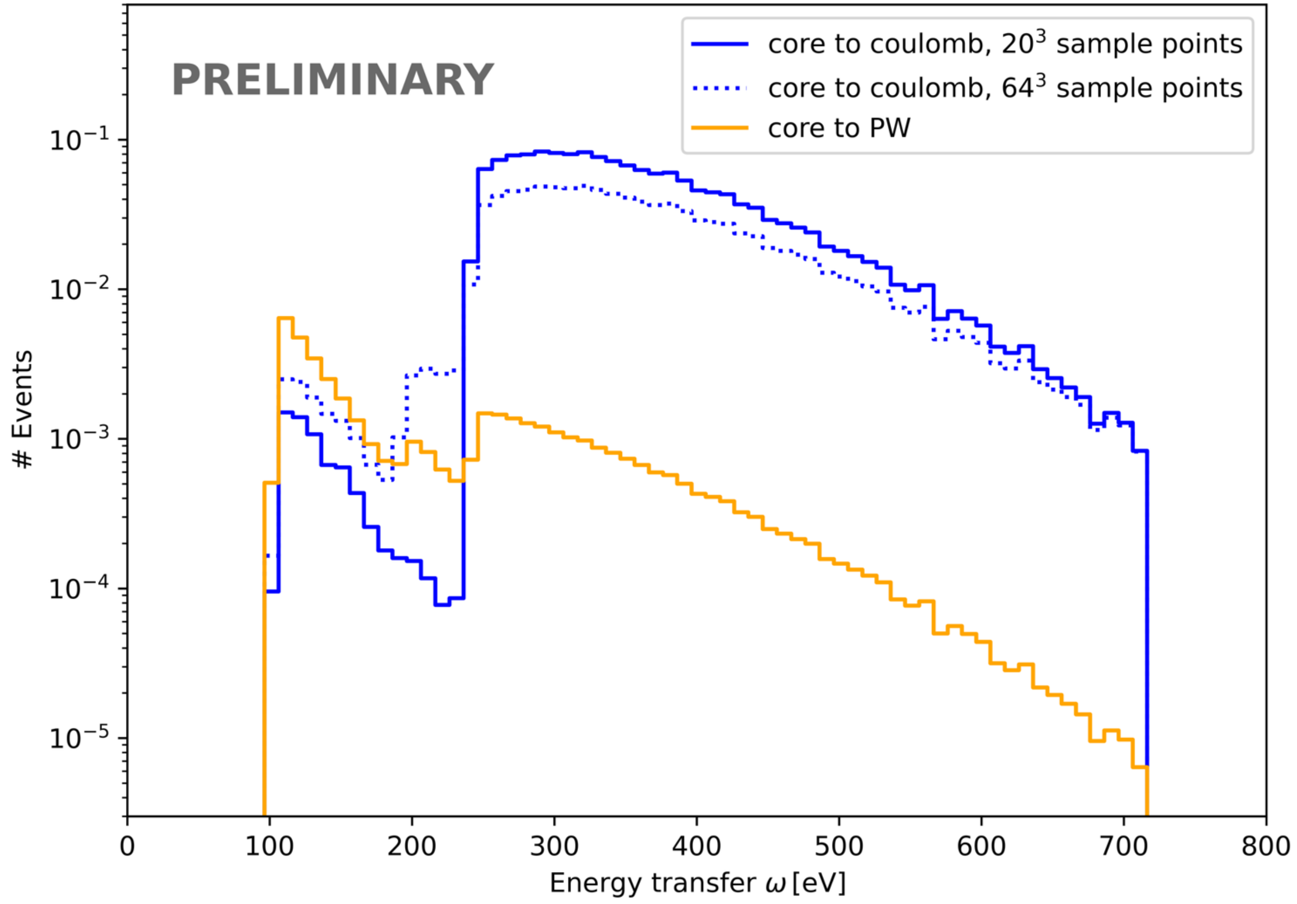

Numerical integration over the unit cell causes problems

How many sample points for a stable result?

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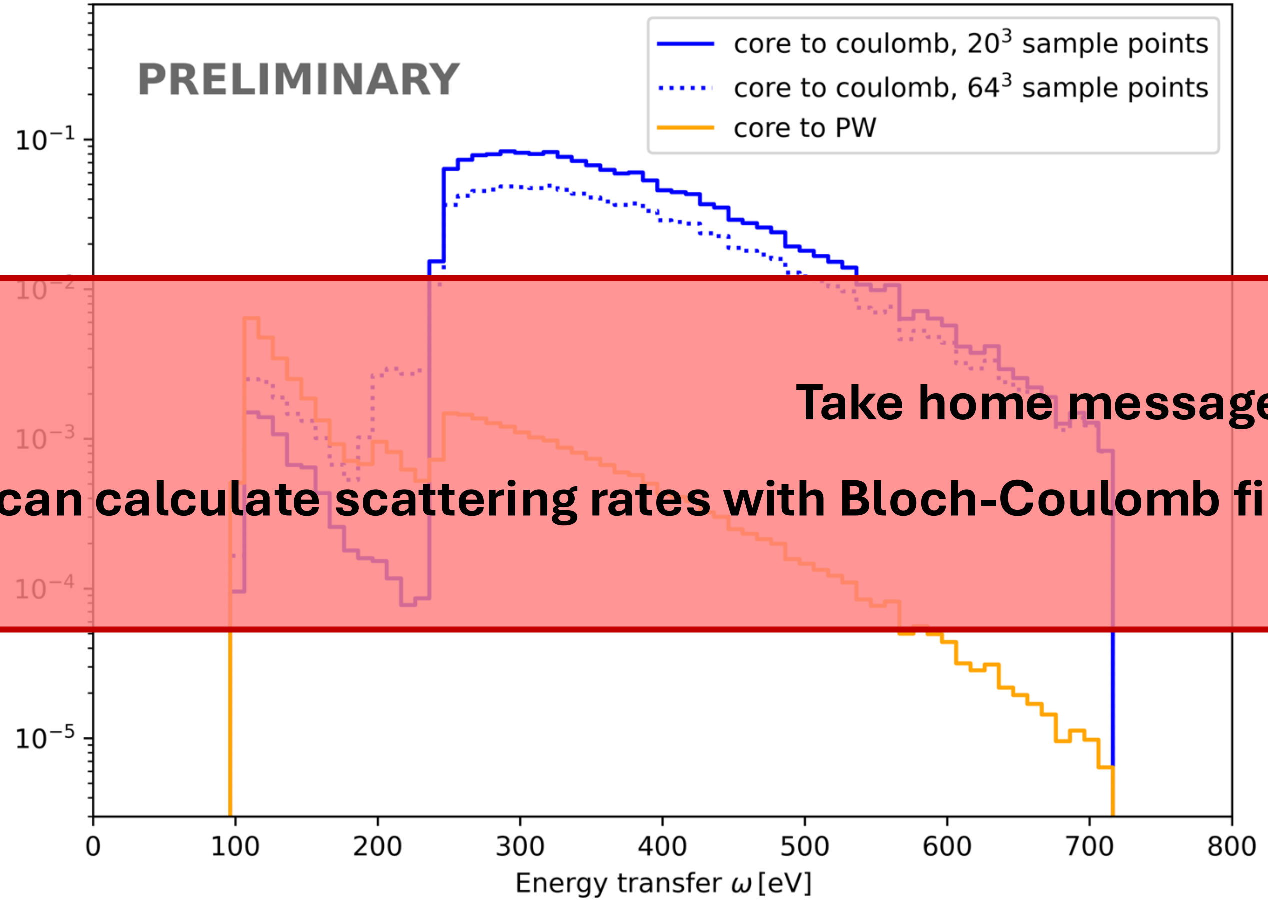

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Take home message:

We can calculate scattering rates with Bloch-Coulomb final states, but more testing is needed!