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

Theresa M. Backes

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

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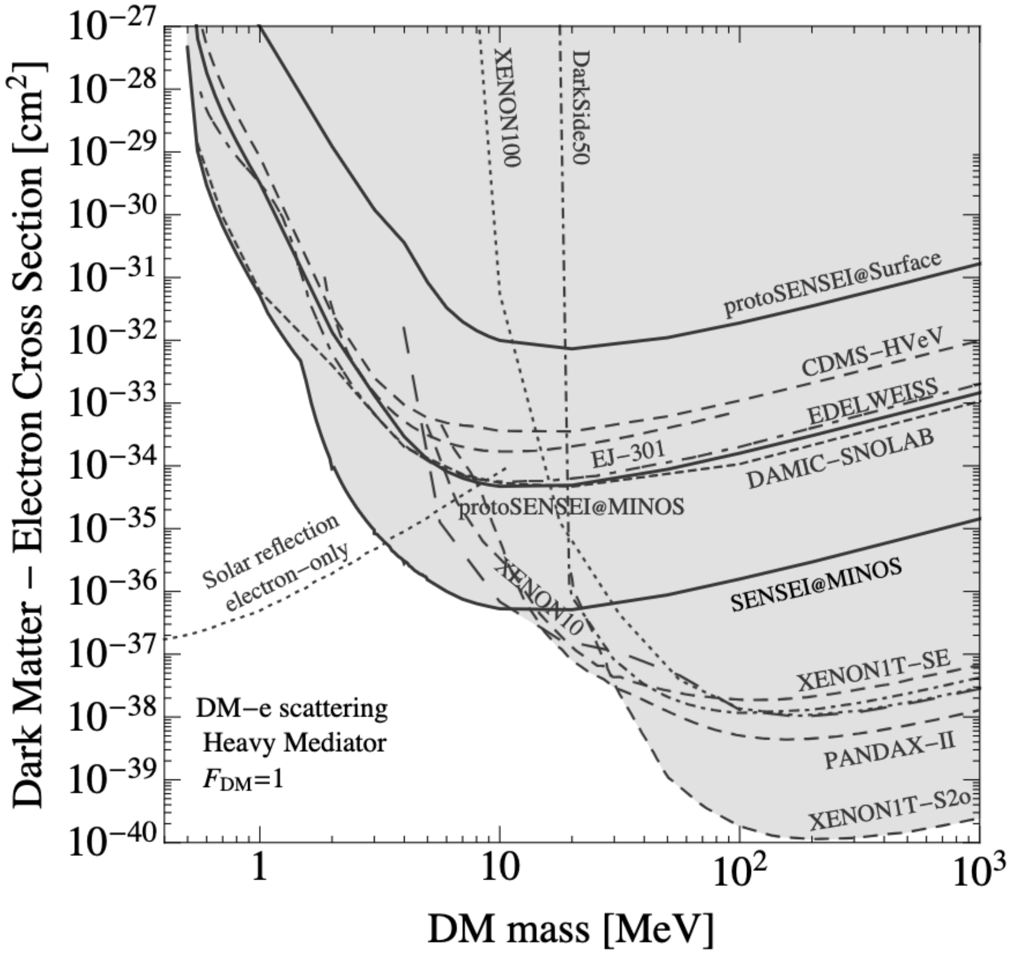
Searching sub-GeV DM with liquid Xenon



Snowmass2021; arXiv:2203.08297

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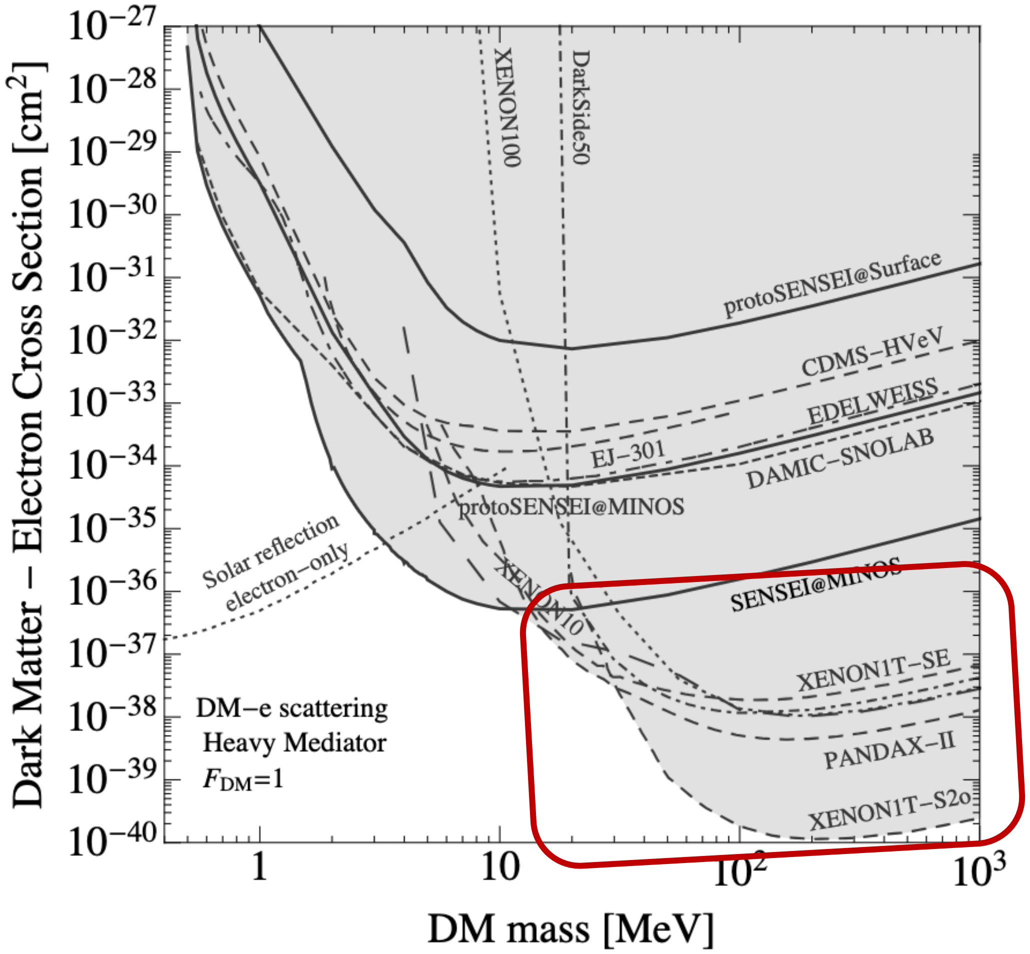

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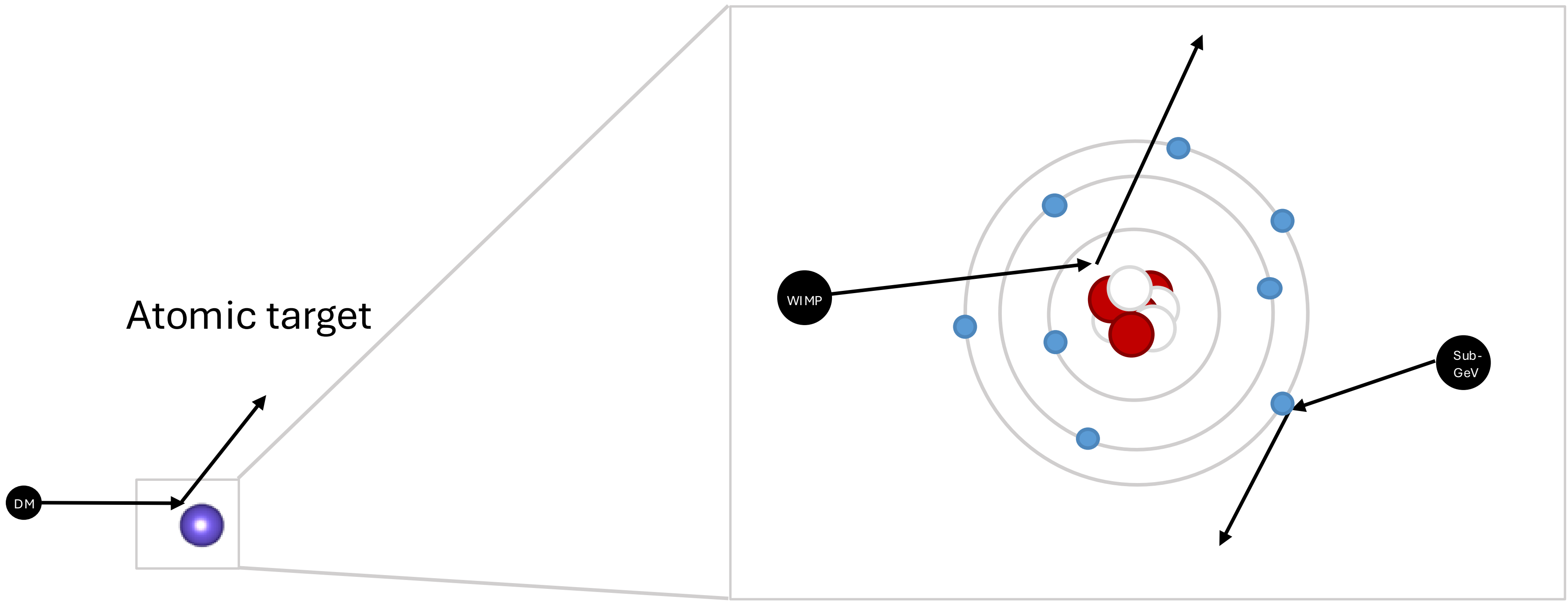
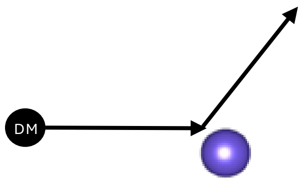
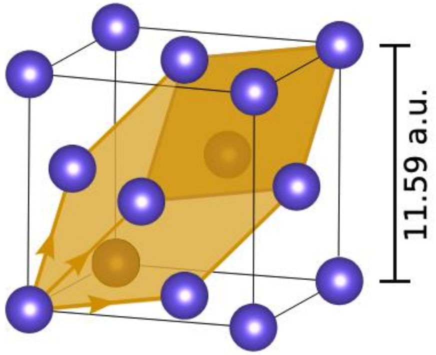


Searching sub-GeV DM with liquid Xenon

Crystal target

Atomic target





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

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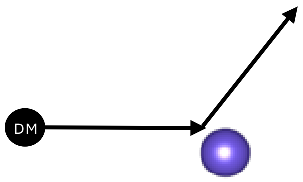

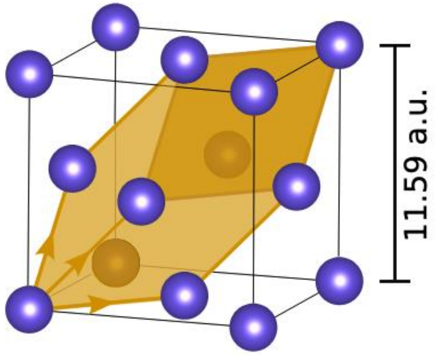

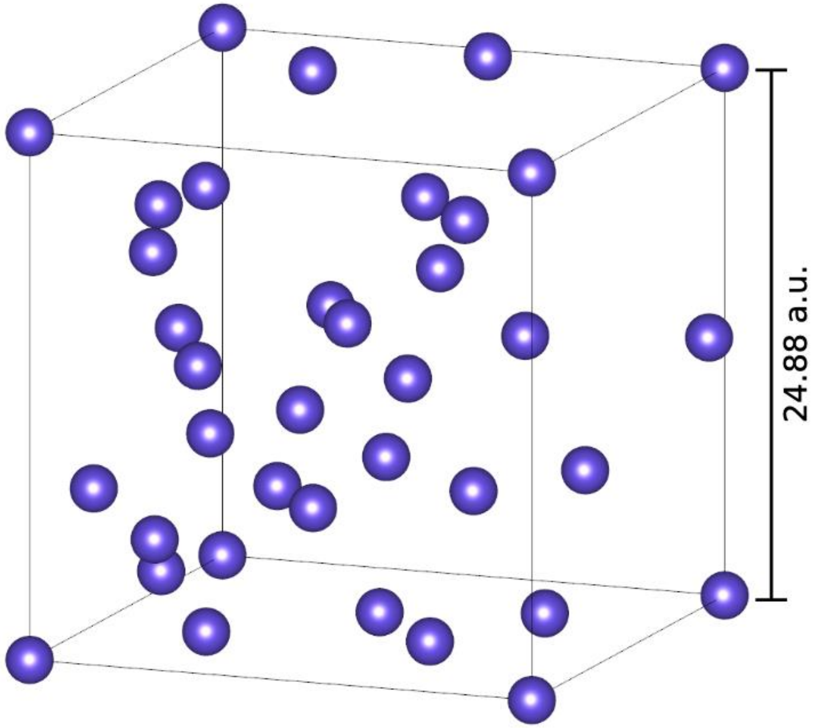

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Electronic states in EXCEED-DM

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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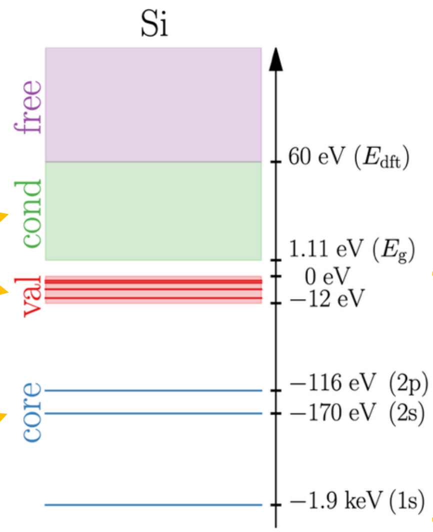
Crystal targets

Single plane waves

DFT calculated

Slater type orbitals (STO's)



Final states

Initial states

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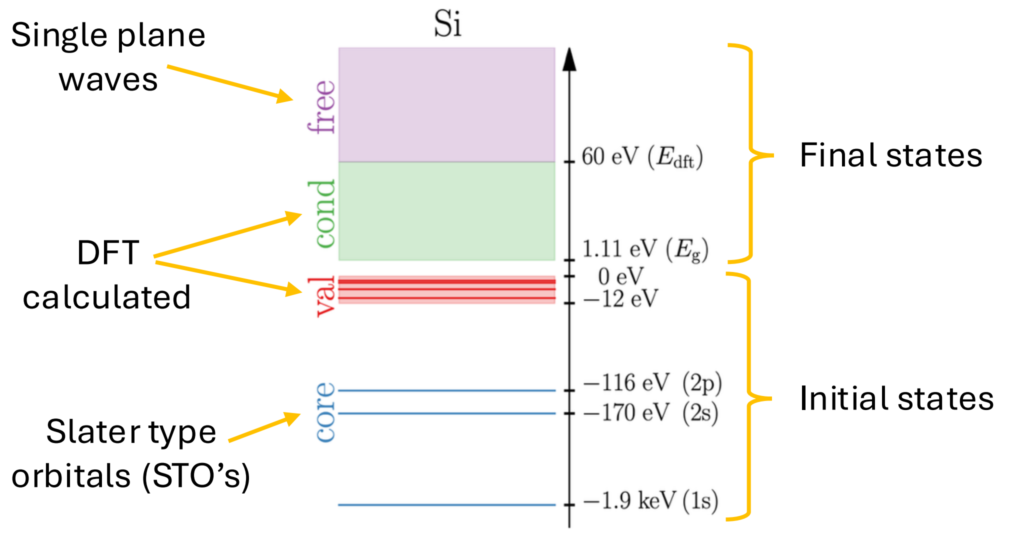


Absorption in **atomic targets**:
G. Krnjaic, T. Trickle; doi:10.1103/PhysRevD.108.015024

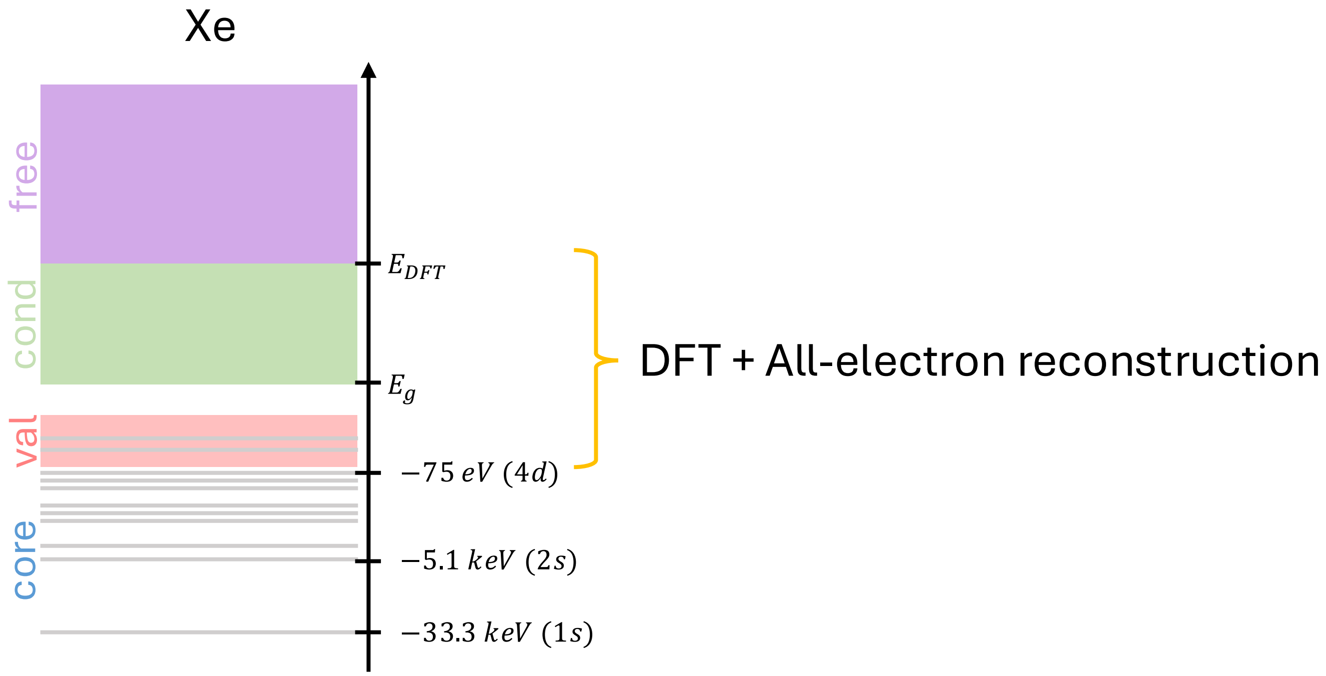
Coulomb states

↑

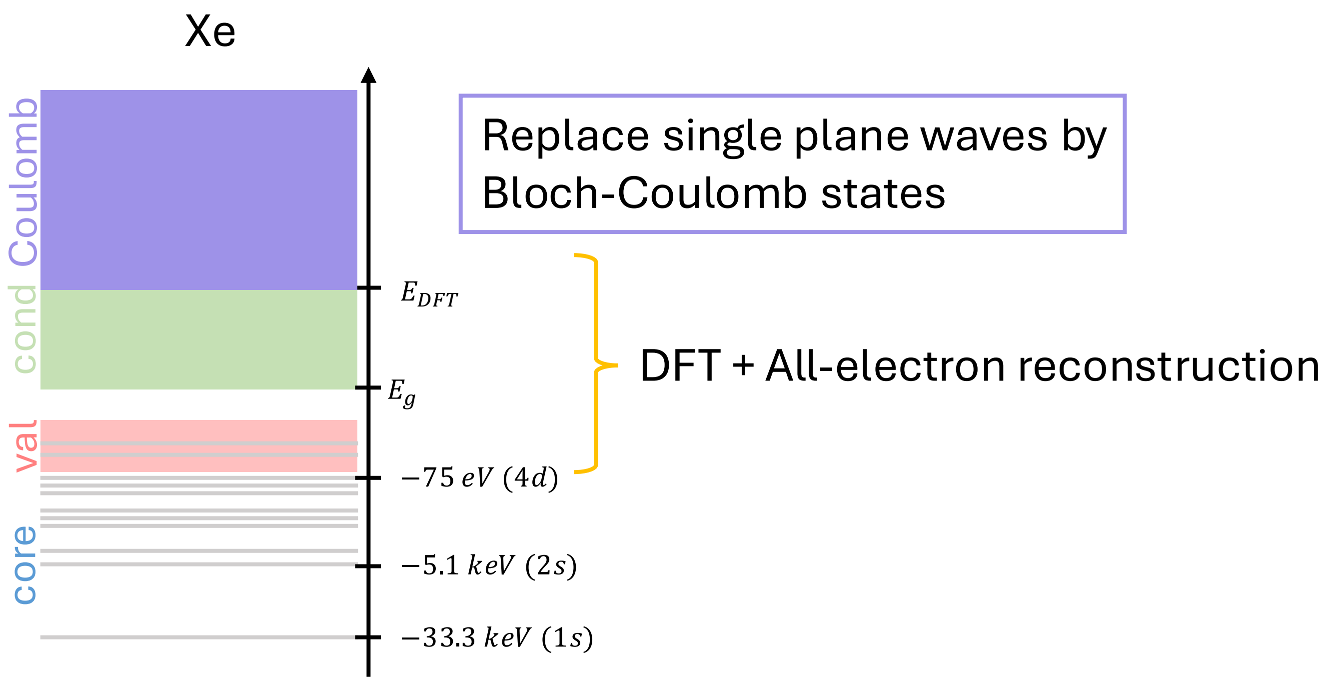
Core states (STO's)

Isolated Atoms

Electronic states of Xenon



Electronic states of Xenon



Replace single plane waves by Bloch-Coulomb states

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New Coulomb states

Positive energy solutions of the Schrödinger equation for isolated atoms:

$$\Psi_{p_f l m}(\mathbf{x}) = R_{\eta l}(x, p_f) Y_l^m(\Omega_{\mathbf{x}})$$

G. Krnjaic, T. Trickle; doi:10.1103/PhysRevD.108.015024

Unbound hydrogen-like orbitals

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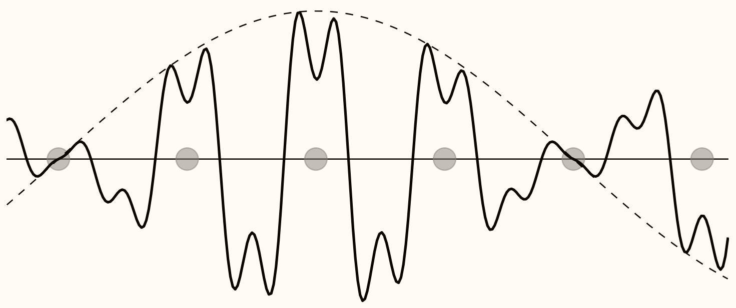
G. Krnjaic, T. Trickle; doi:10.1103/PhysRevD.108.015024

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

New Coulomb states

Positive energy solutions of the Schrödinger equation for isolated atoms:

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

$$\Psi_{\mathbf{p}_f}(\mathbf{x}) = \frac{1}{\sqrt{V}} e^{i\mathbf{p}_f\cdot\mathbf{x}} \sum_{\mathbf{r}} \sum_{\mathbf{x}_{eq}} e^{i\mathbf{p}_f\cdot(\mathbf{x}-\mathbf{r}-\mathbf{x}_{eq})} \cdot 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l e^{i\sigma_l} R_{\eta l}(x - r - x_{eq}, p_f) \cdot Y_l^m(\Omega_{\mathbf{x}-\mathbf{r}-\mathbf{x}_{eq}}) Y_l^m(\Omega_{\mathbf{p}_f})$$

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

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$$= \frac{1}{\sqrt{V}} e^{i\mathbf{p}_f\cdot\mathbf{x}} \sum_{\mathbf{r}} \sum_{\mathbf{x}_{eq}} e^{i\mathbf{p}_f\cdot(\mathbf{x}-\mathbf{r}-\mathbf{x}_{eq})} \sum_{l=0}^{\infty} i^l e^{i\sigma_l} (2l+1) R_{\eta l}(x - r - x_{eq}, p_f) P_l(\hat{\mathbf{y}} \cdot \hat{\mathbf{p}}_f)$$

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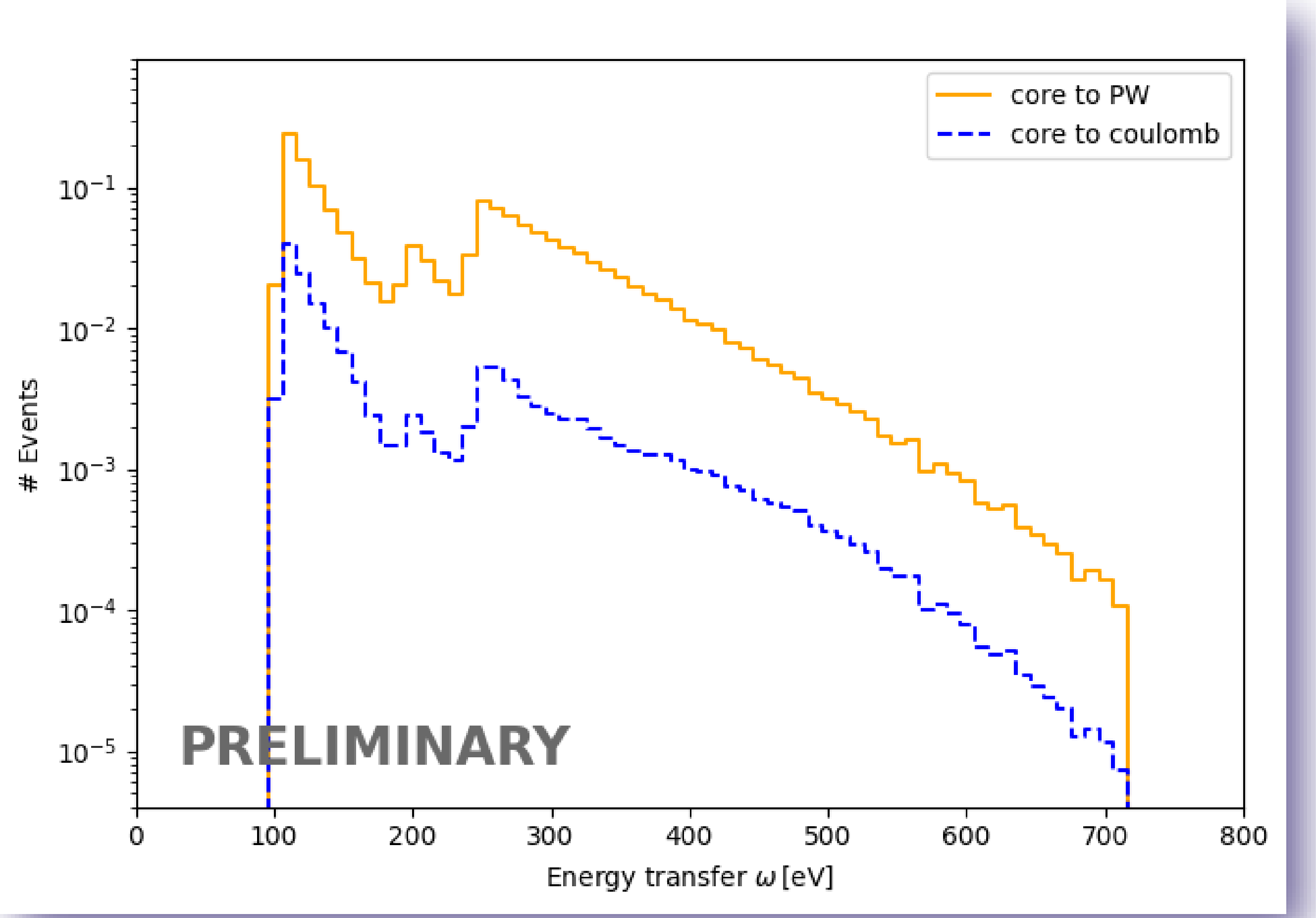
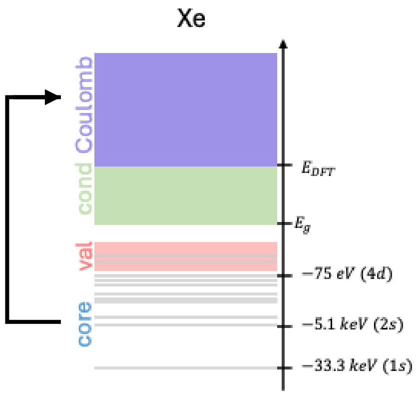
Tests with crystalline Xenon

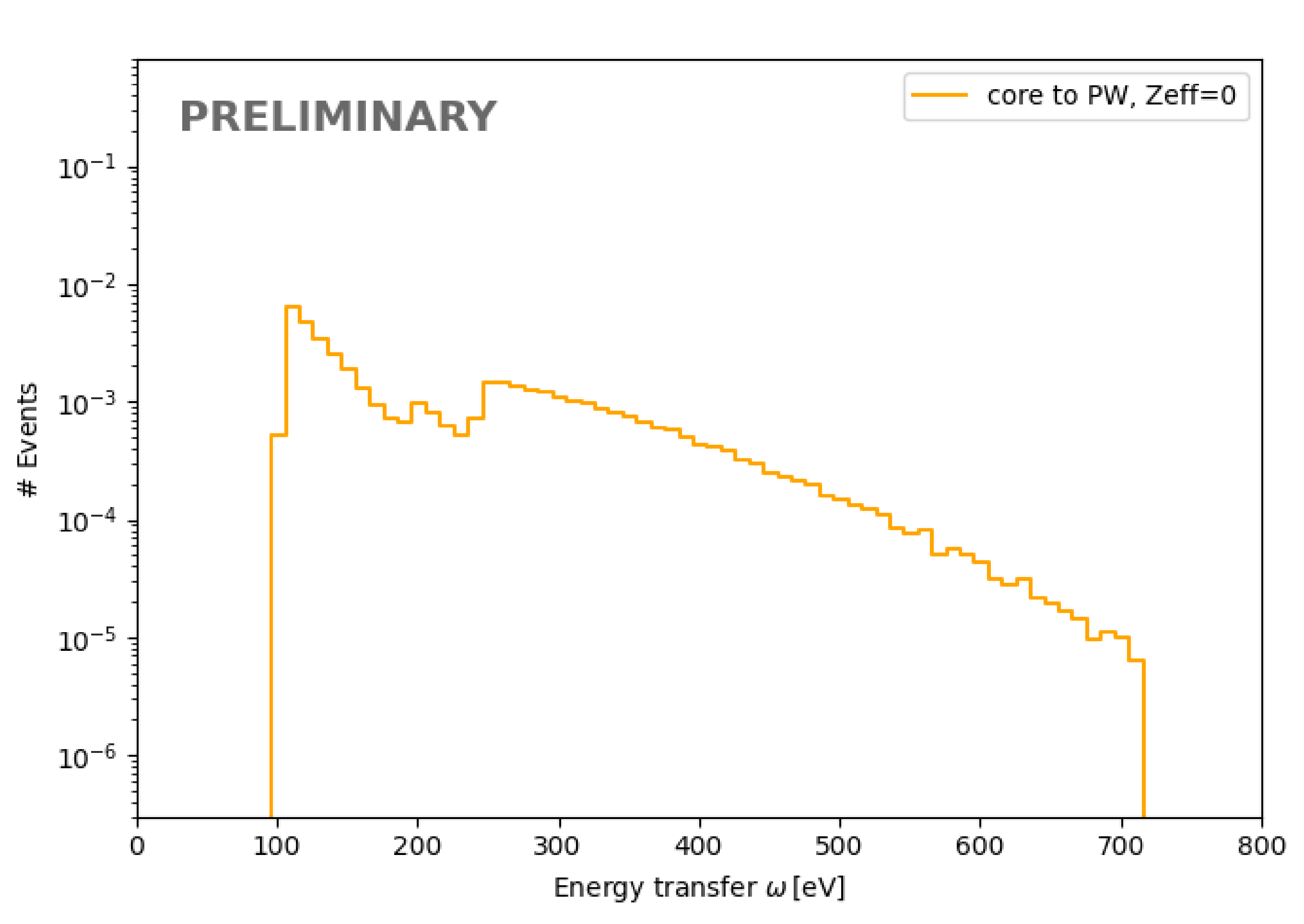




Sanity check $Z_{eff} = 0$

$$\Psi_{\mathbf{p}_f}(\mathbf{x}) = \frac{1}{\sqrt{V}} e^{i\mathbf{p}_f\cdot\mathbf{x}} \sum_{\mathbf{r}} \sum_{\mathbf{x}_{eq}} e^{i\mathbf{p}_f\cdot(\mathbf{x}-\mathbf{r}-\mathbf{x}_{eq})}$$
$$\cdot \sum_{l=0}^{\infty} i^l e^{i\sigma_l} R_{\eta l}(x - r - x_{eq}, p_f)$$
$$\cdot (2l+1) P_l(\hat{\mathbf{y}} \cdot \hat{\mathbf{p}}_f)$$

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



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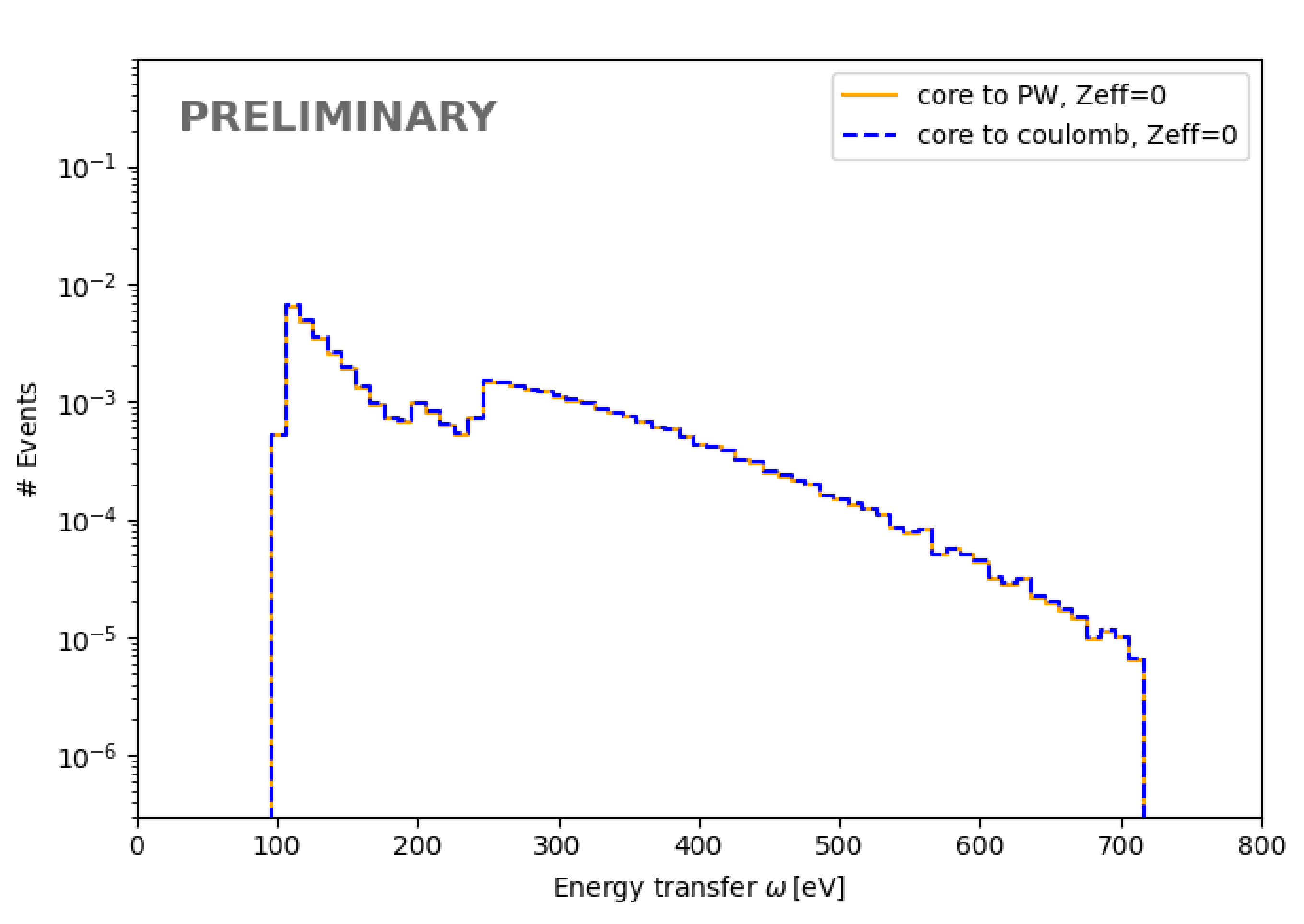

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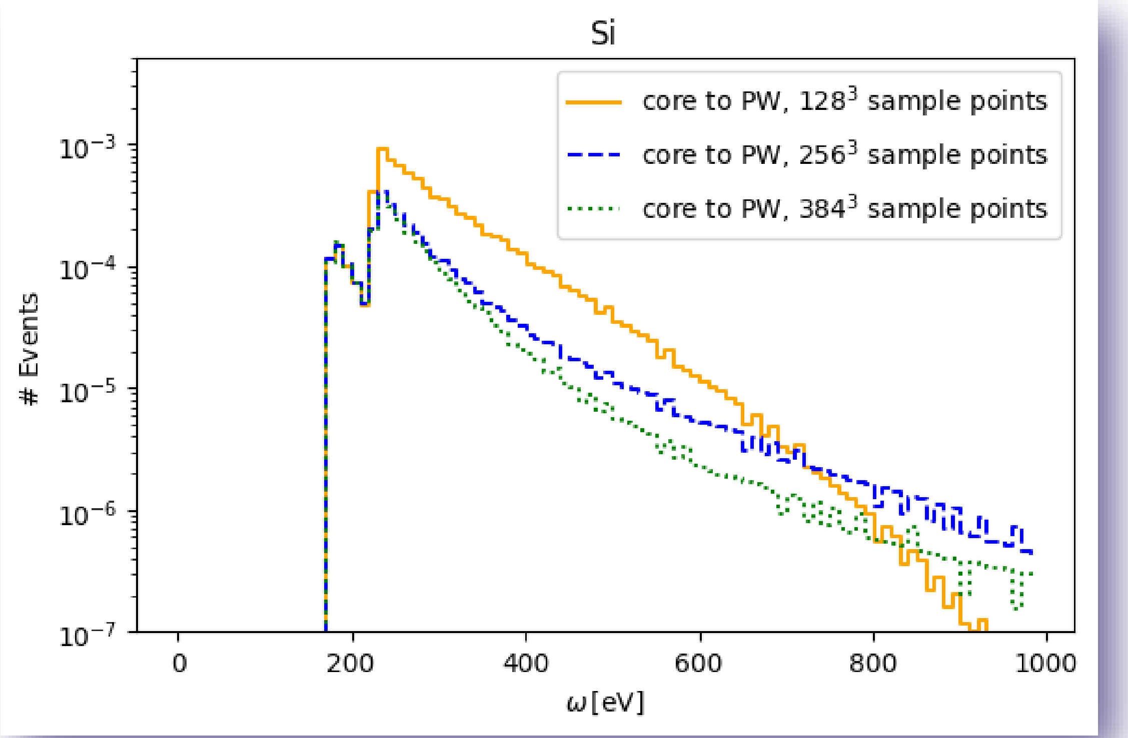
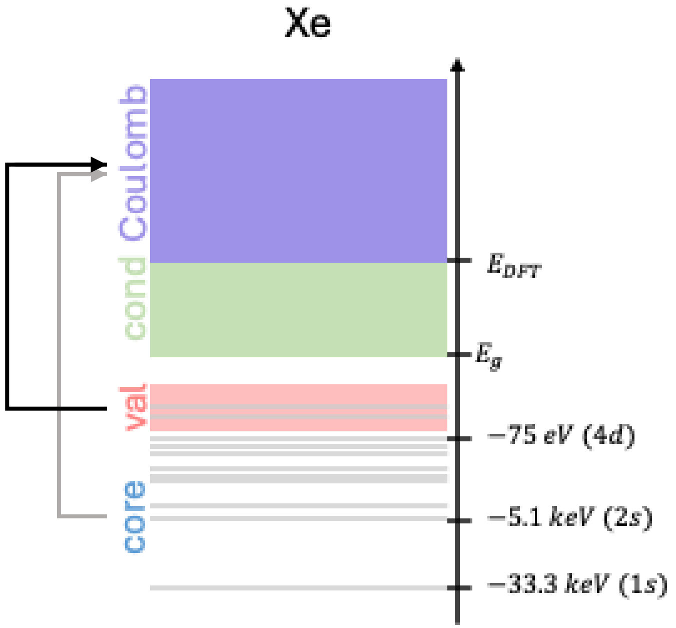
Next steps



- Check stability with regards to sampling
- Add valence to coulomb state calculations
- Run the calculations for super cells instead of crystalline Xenon

Next steps



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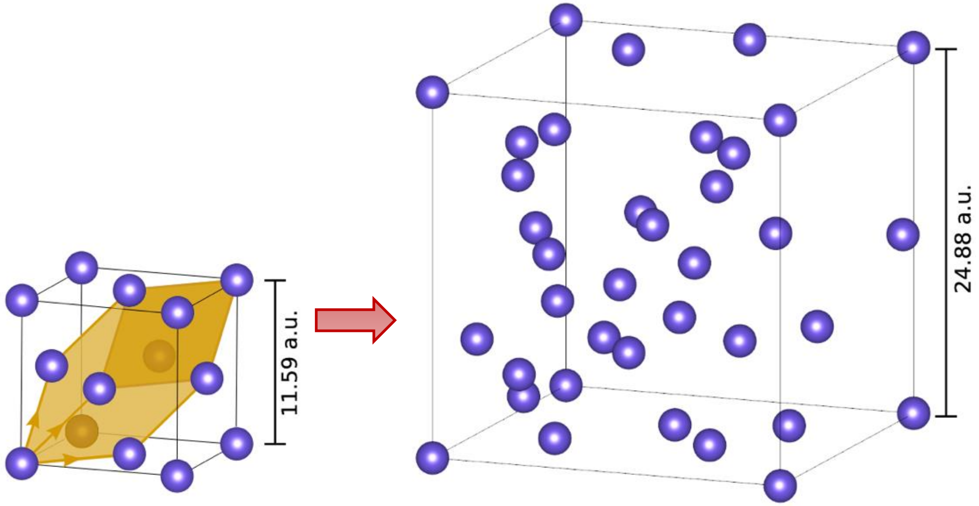

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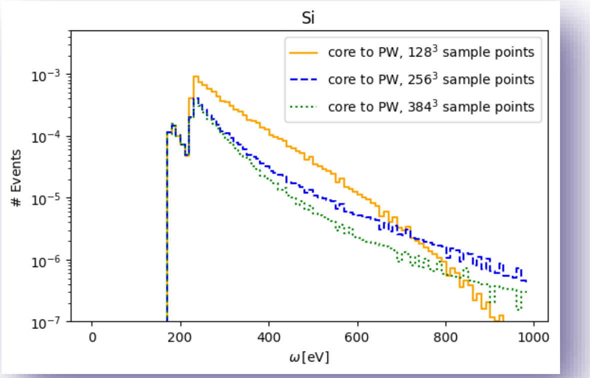

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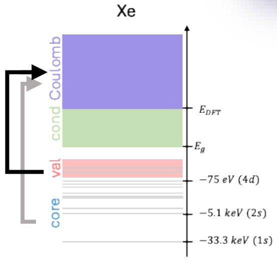

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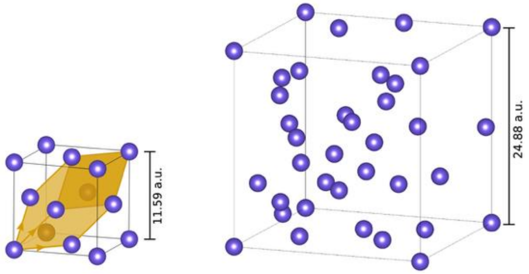

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- Combine all of this with the work on the initial states done by our collaborators