Ab initio all-electron calculation for sub-GeV dark matter direct detection

with emphasis on a new code, Quantum Chemistry Dark (QCDark)

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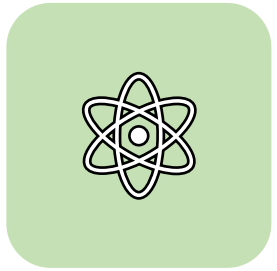
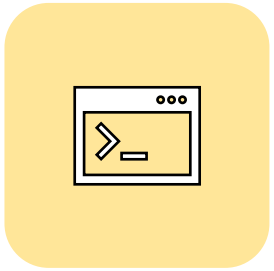
In collaboration with Cyrus Dreyer, Rouven Essig, Marivi Fernandez-Serra, Cheng Zhen

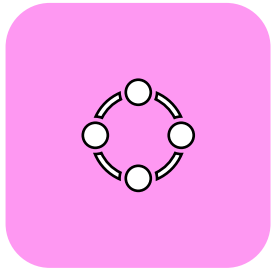
Outline



SUB-GEV DARK MATTER DIRECT DETECTION



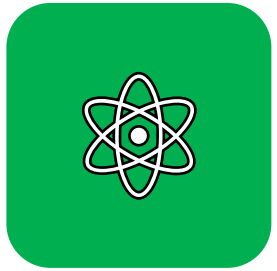
ELECTRONIC EXCITATIONS IN SEMICONDUCTORS



EFFECTS OF INCLUDING CORE ORBITALS

QUANTUM CHEMISTRY DARK (QCDARK)

Outline



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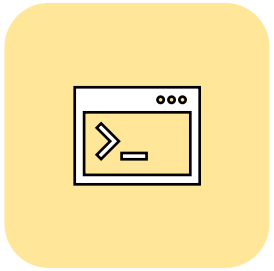

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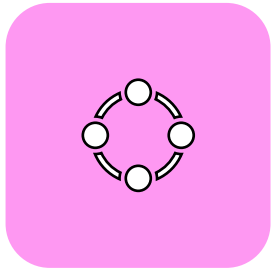
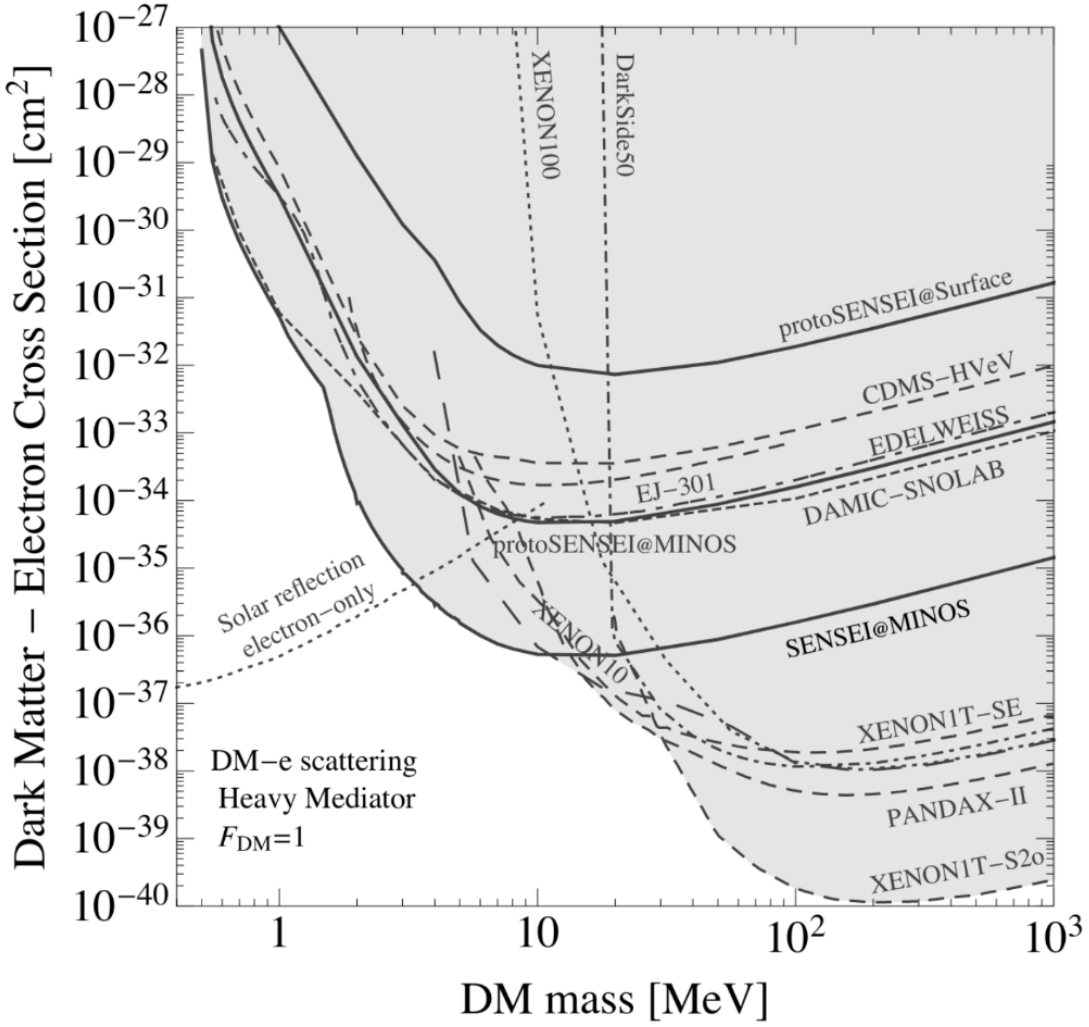
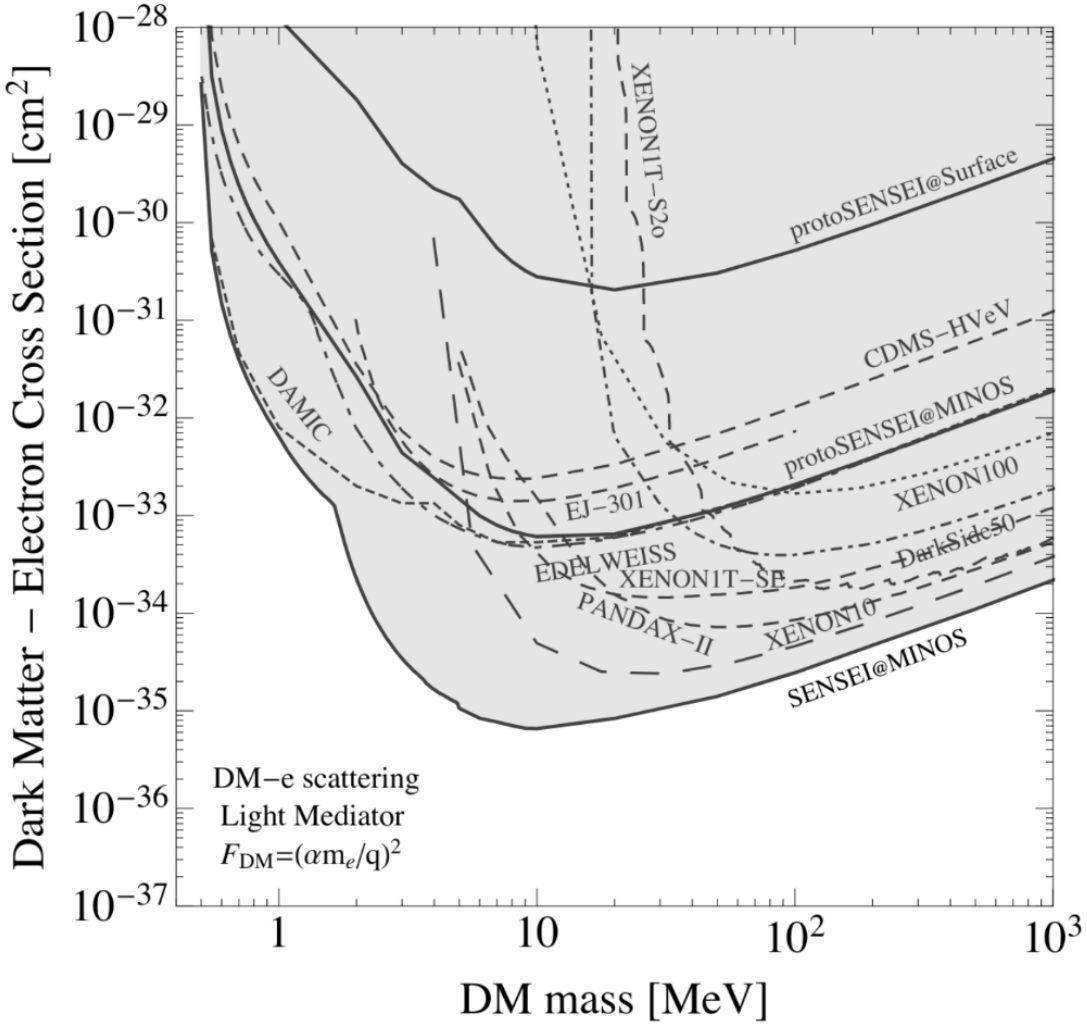


EFFECTS OF INCLUDING CORE ORBITALS

QUANTUM CHEMISTRY DARK (QCDARK)

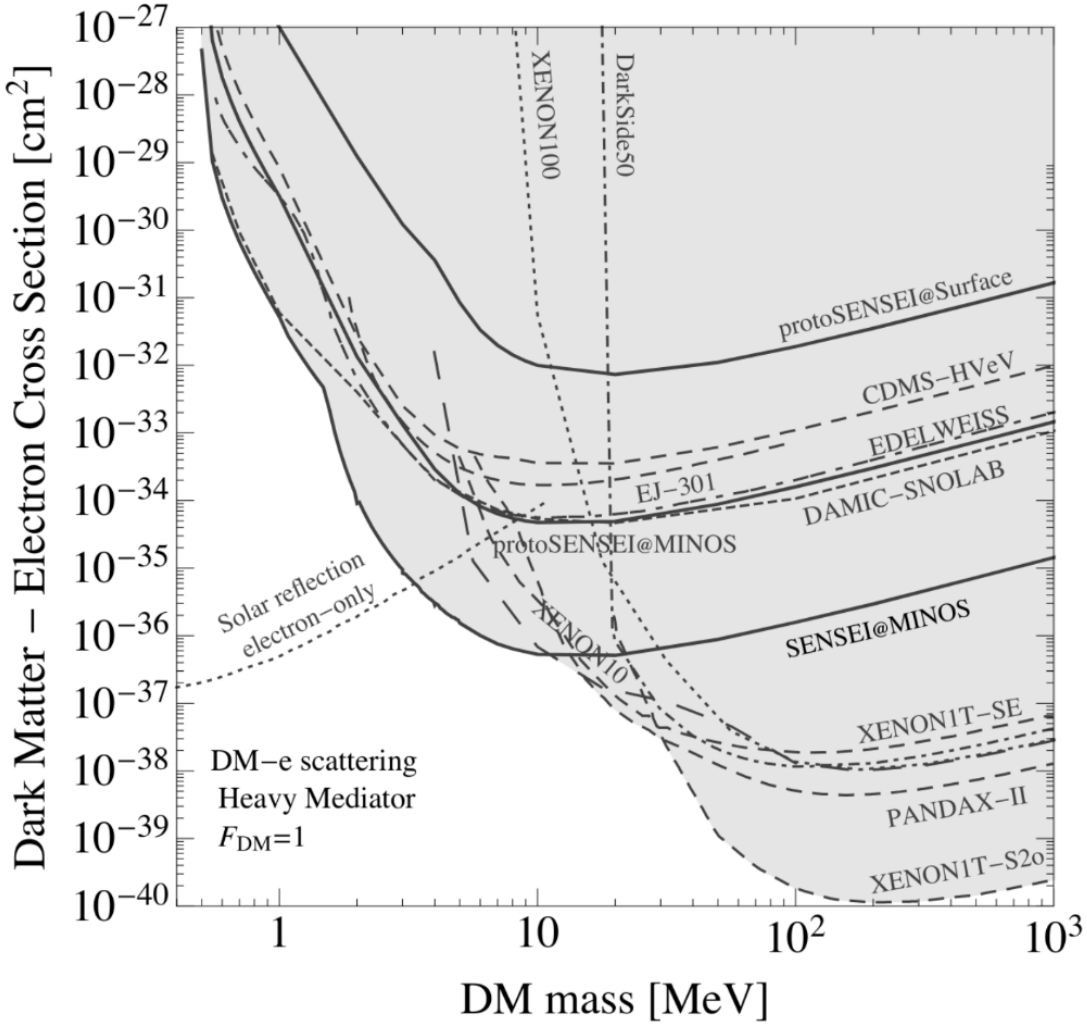
Experiments probing sub-GeV dark matter–electron scattering

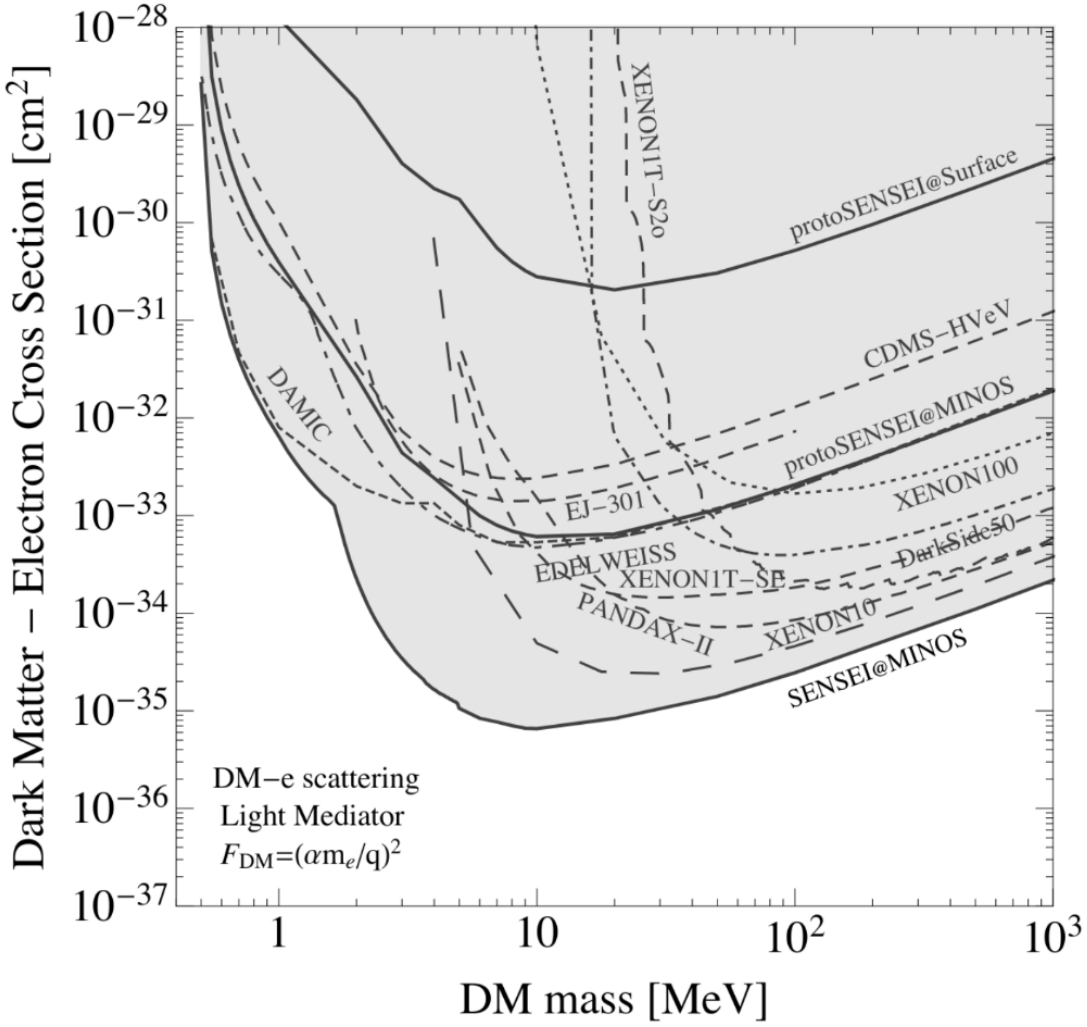




Essig et al, Snowmass2021 Cosmic Frontier (2203.08297)

Experiments probing sub-GeV dark matter–electron scattering

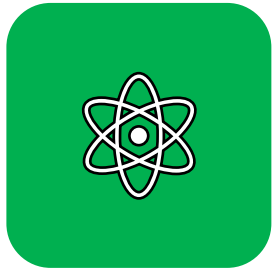




Need to understand the theoretical rates well!

Essig et al, Snowmass2021 Cosmic Frontier (2203.08297)

Outline



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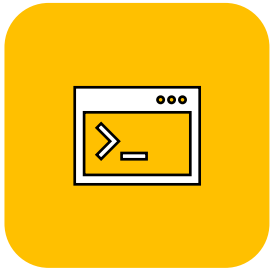

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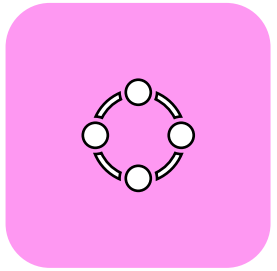
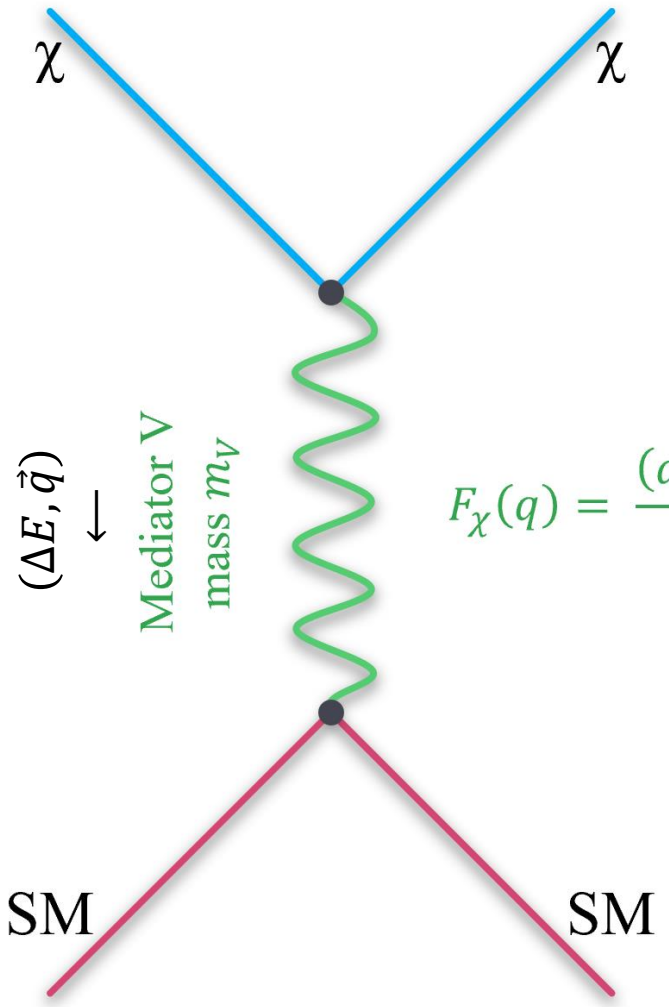


EFFECTS OF INCLUDING CORE ORBITALS

QUANTUM CHEMISTRY DARK (QCDARK)

Dark matter–electron scattering rates



$$F_\chi(q) = \frac{(\alpha m_e)^2 + m_V^2}{q^2 + m_V^2}$$

$$\frac{dR}{d\Delta E} = N_T \int d^3q \frac{1}{q} \int d^3v \, n_\chi v \, f(\vec{v}) \, \frac{d\,\sigma}{d\Delta E},$$

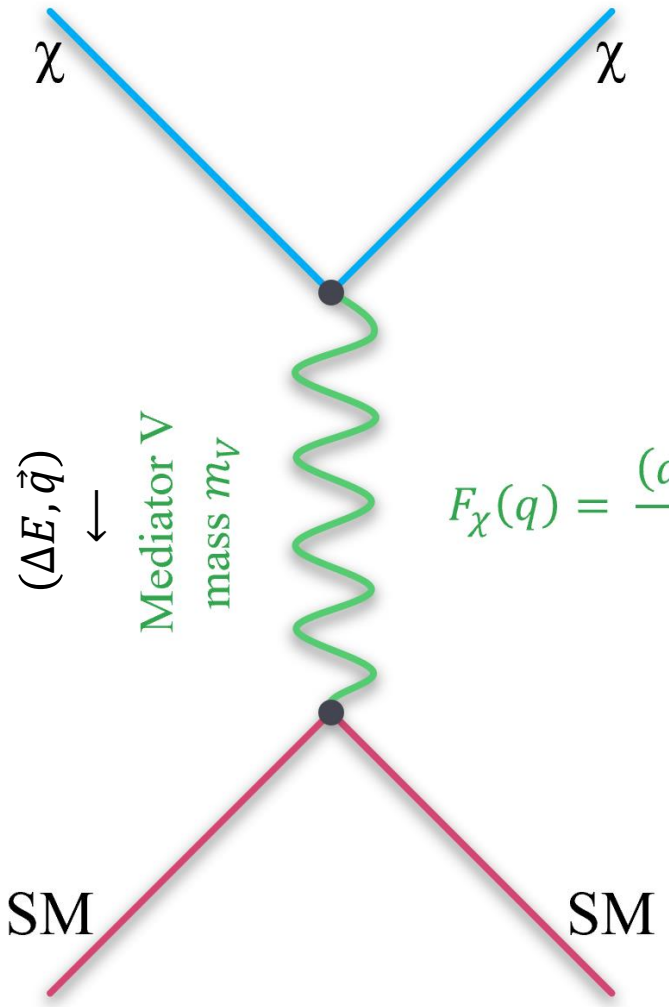
Astrophysical DM flux

DM interaction with material response

$$\frac{d\sigma}{d\Delta E} \sim \frac{\bar{\sigma}}{2v^2\mu^2} \left|F_\chi(q)\right|^2 |F_{\text{material}}(q, \Delta E)|^2 \Theta(v - v_{\text{min}})$$

QEDark: Essig, Fernandez-Serra, Mardon, Soto, Yu (1509.01598)

Dark matter–electron scattering rates



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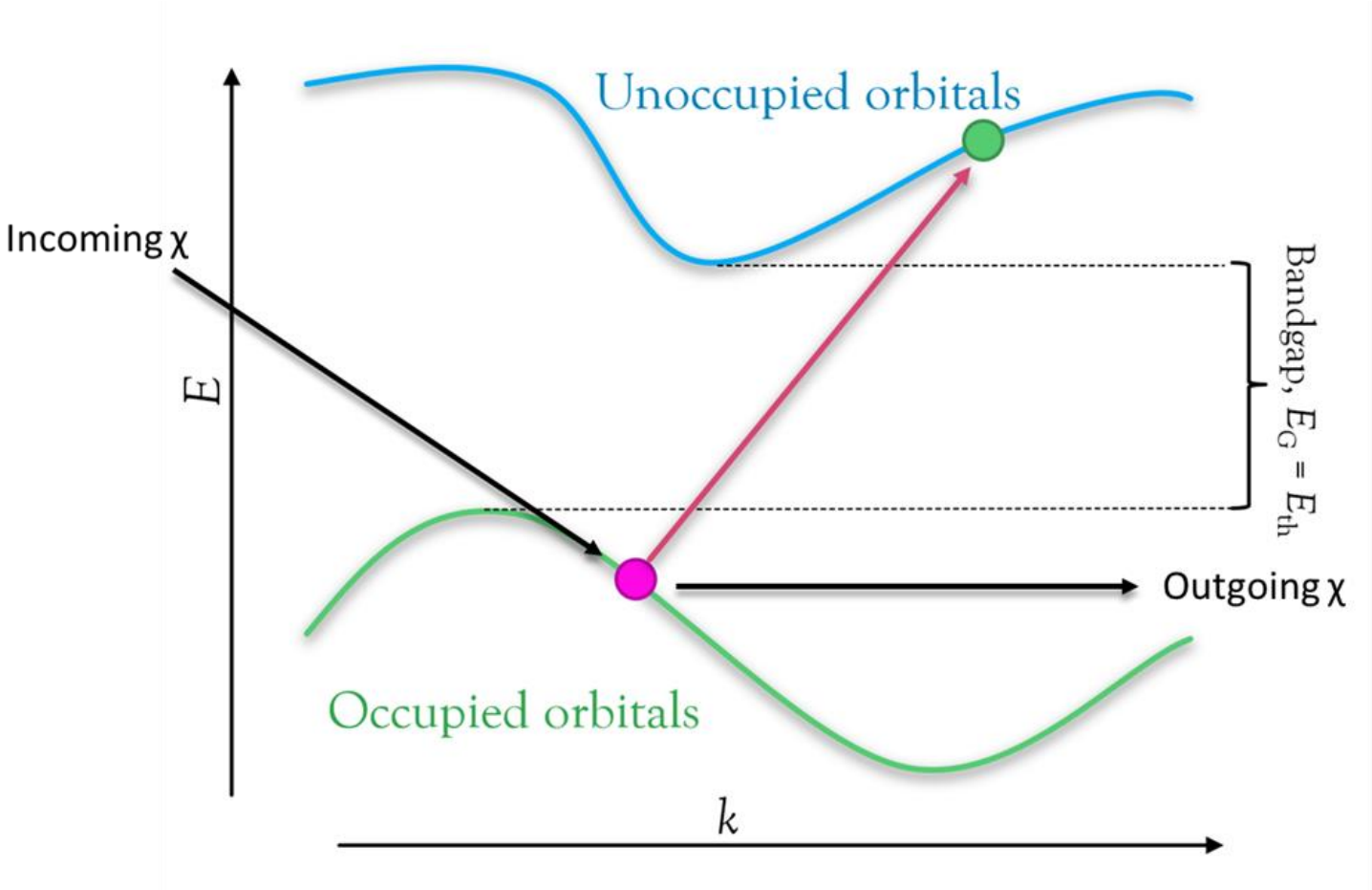
We calculate the target material response for semiconductors

QEDark: Essig, Fernandez-Serra, Mardon, Soto, Yu (1509.01598)

Material response in crystals, crystal form factor



- DM strikes electron in any occupied band.
- electron gets excited, leaving hole behind!

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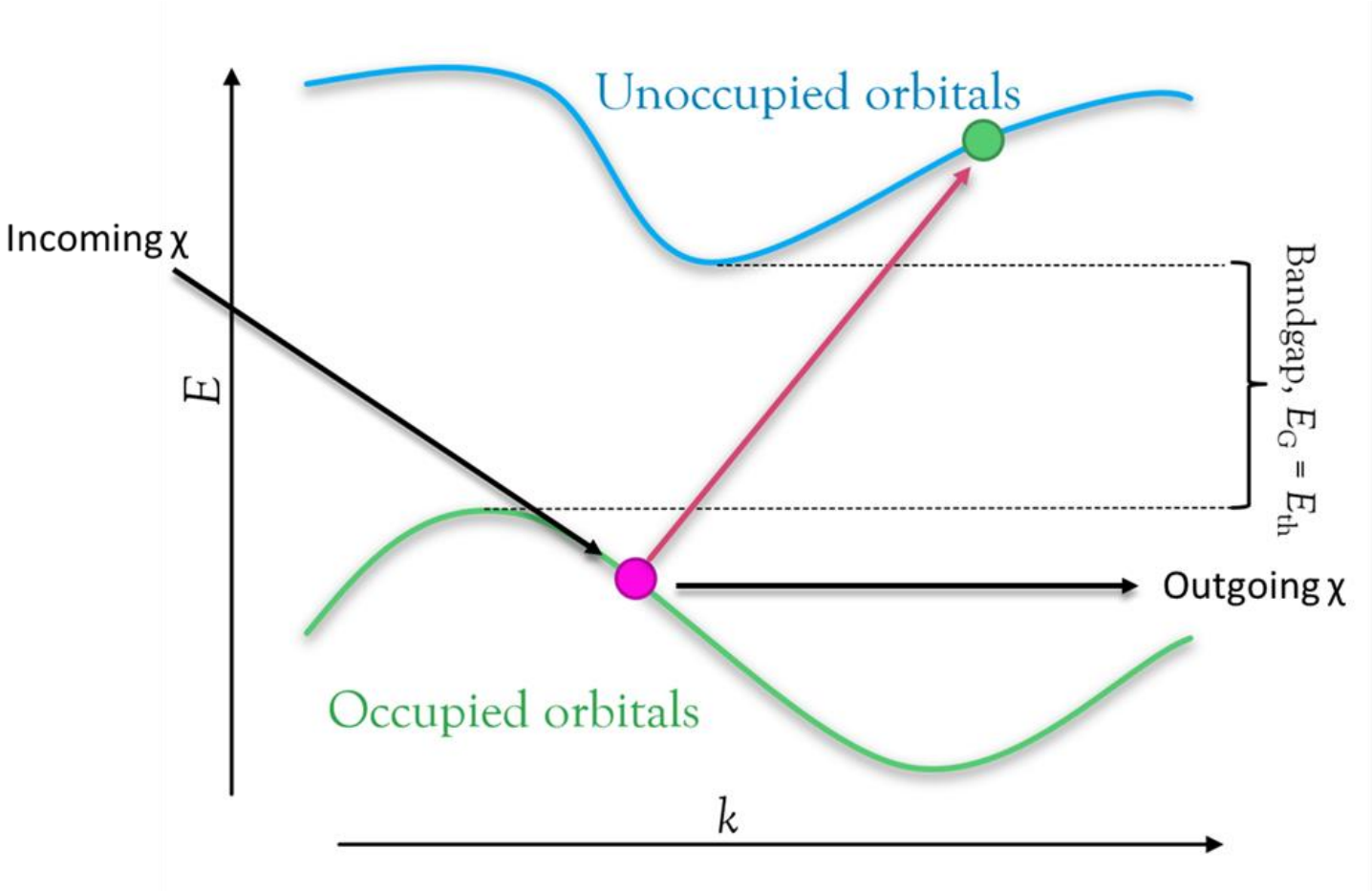

- DM strikes electron in any occupied band.
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- $\left|f_{\text{crystal}}(q, \Delta E)\right|^2 \sim$ total transition probability of exciting an electron
  from any occupied shell
  to any unoccupied shell.

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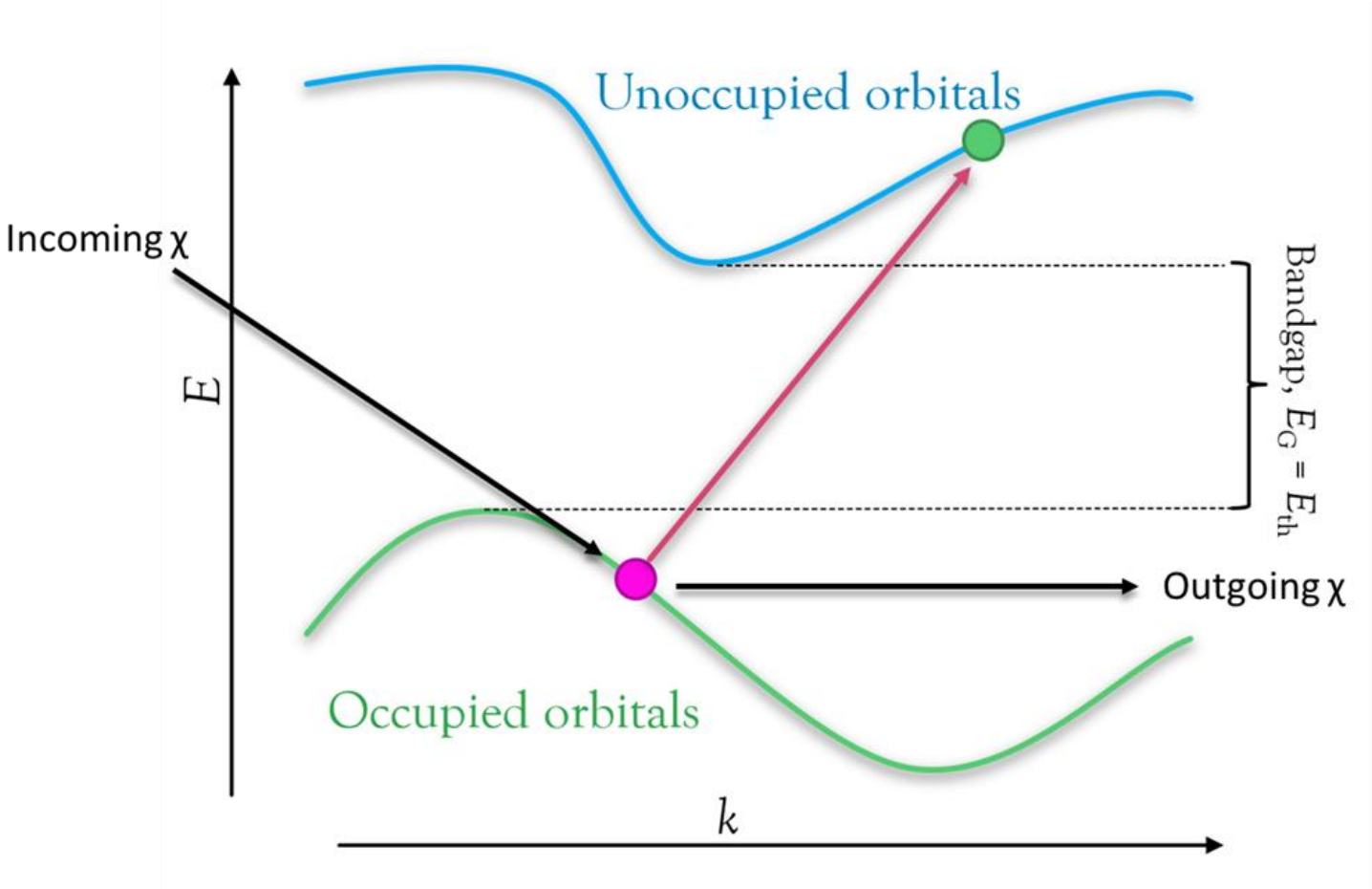
Material response in crystals, crystal form factor



- DM strikes electron in any occupied band.
- electron gets excited, leaving hole behind!

We call this crystal form factor!

- $\left|f_{\text{crystal}}(q, \Delta E)\right|^2$ ~ total transition probability of exciting an electron
  from any occupied shell
  to any unoccupied shell.

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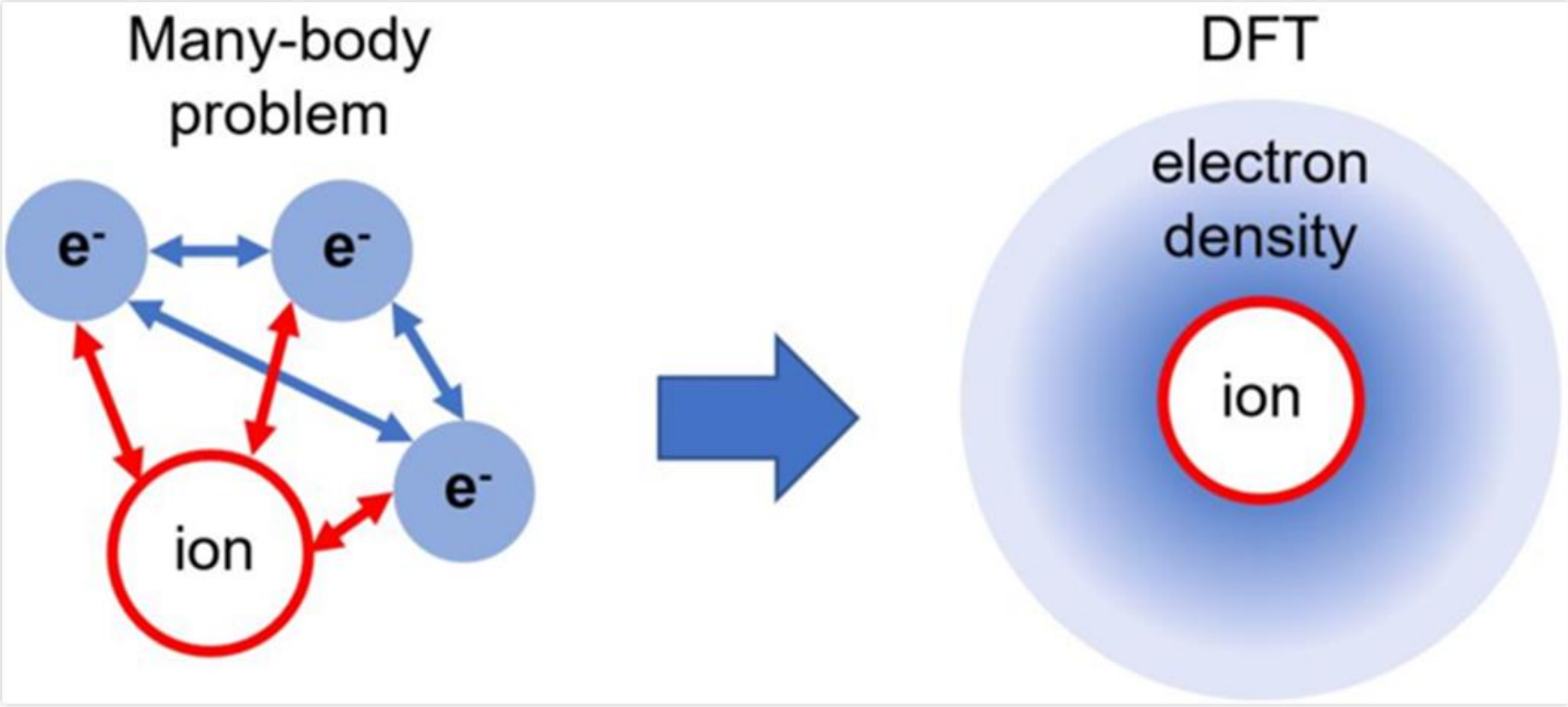
Calculating crystal form factor

- Need to calculate electron wavefunctions in crystals – many body problem.
- We use density functional theory (DFT)

  → converts many body problem to non-linear single electron problem.
- Generally, use plane waves as basis for calculating wavefunctions.



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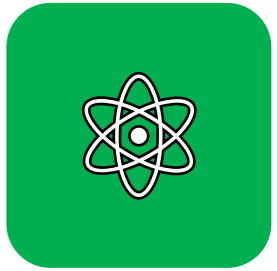
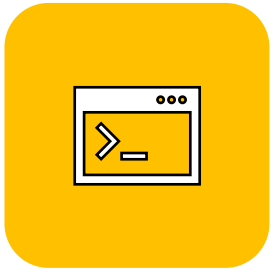
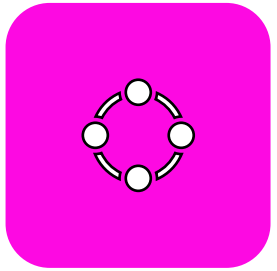


SUB-GEV DARK MATTER DIRECT DETECTION



ELECTRONIC EXCITATIONS IN SEMICONDUCTORS

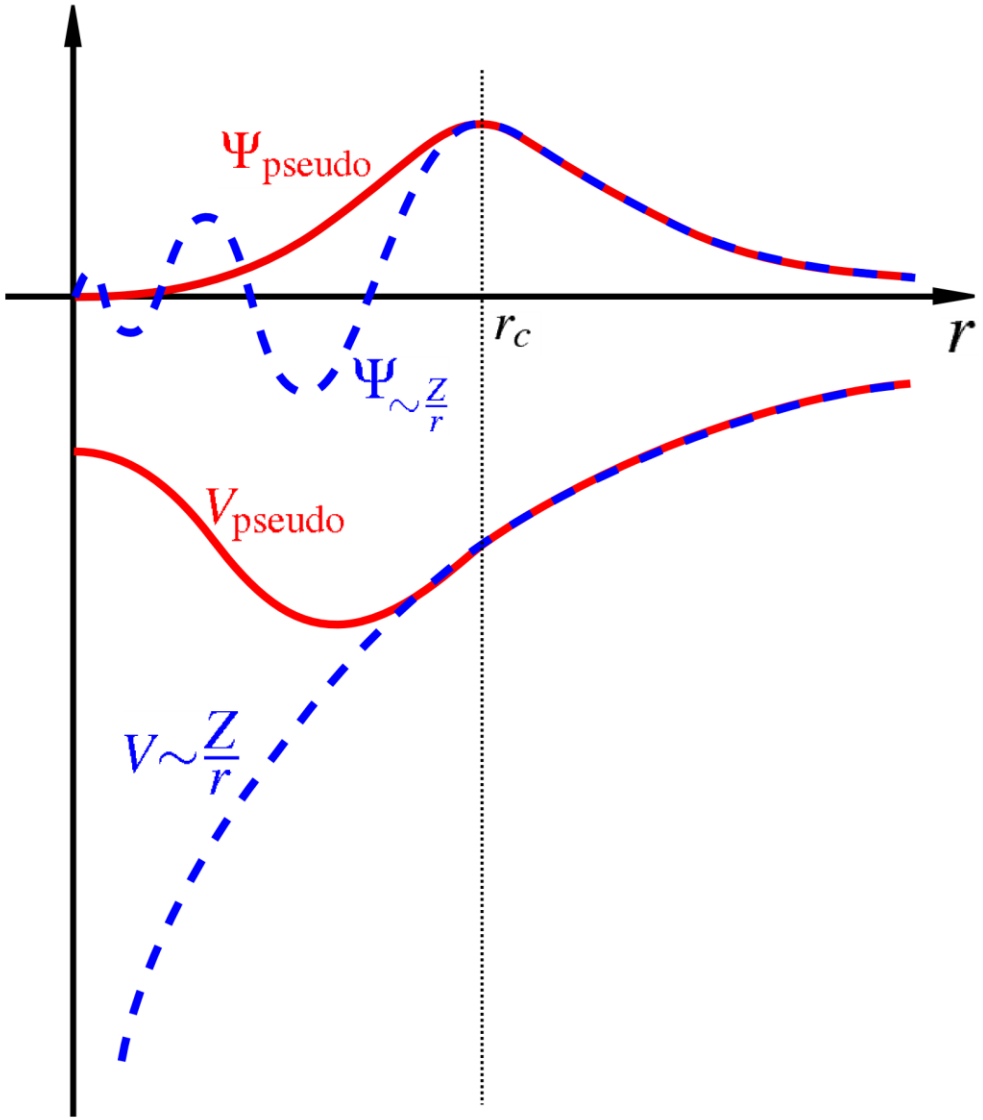


EFFECTS OF INCLUDING CORE ORBITALS

QUANTUM CHEMISTRY DARK (QCDARK)

Pseudopotentials

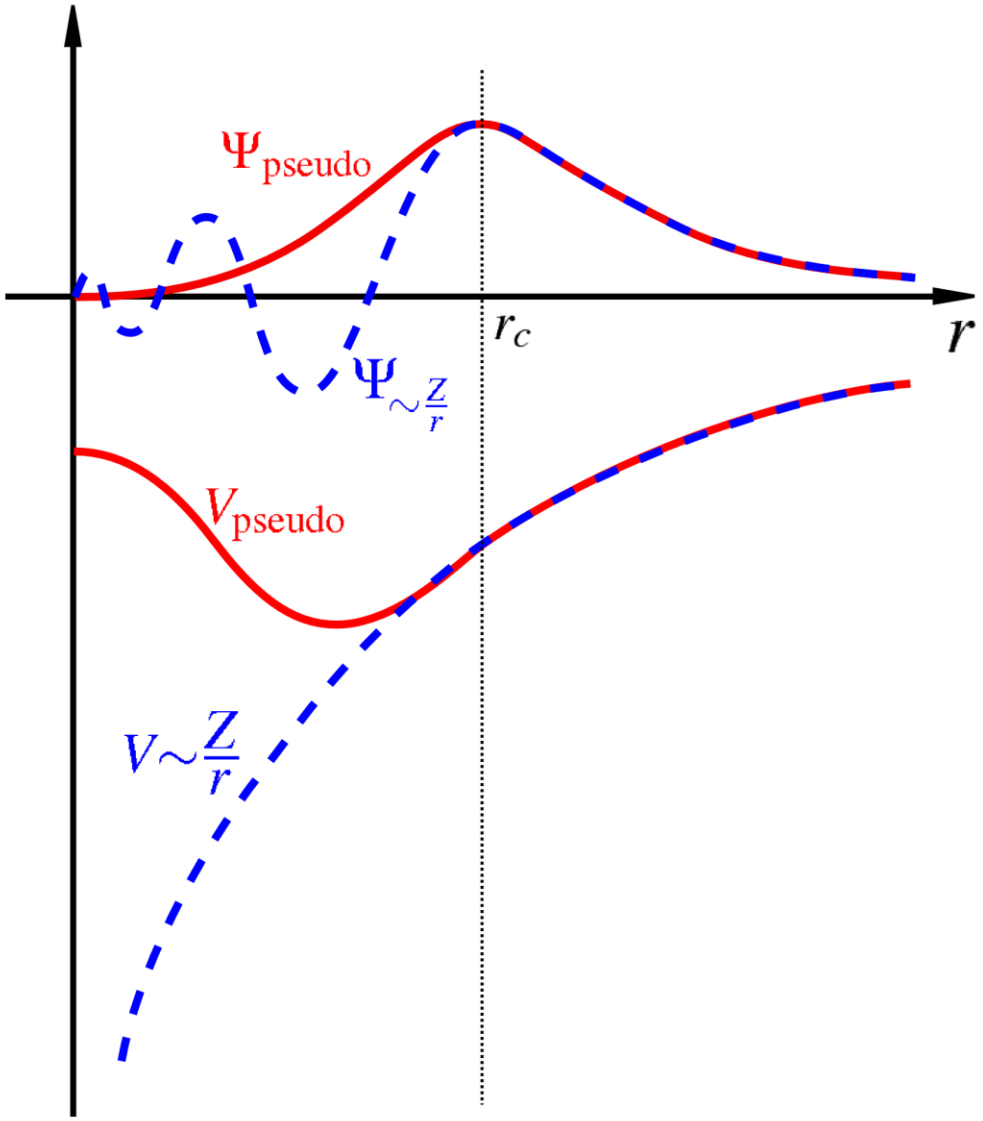
- Core electrons do not participate in bonding and do not get excited.
  - QEDark: models them with an effective potential.
- BUT: this leads to wrong wavefunctions for valence electrons at small radii (large momenta).



QEDark: Essig, Fernandez-Serra, Mardon, Soto, Yu (1509.01598)
EXCEED-DM: Griffin, Inzani, Trickle, Zhang, Zurek (2105.09567), Trickle (2210.14917)

Inclusion of core orbitals, *all–electron effects*

- Inclusion of core orbitals
  → corrects to valence and conduction bands near nuclei
  → *(all–electron effects)*
- EXCEED-DM adds core electrons after pseudopotential calculation
  → all–electron *reconstruction*



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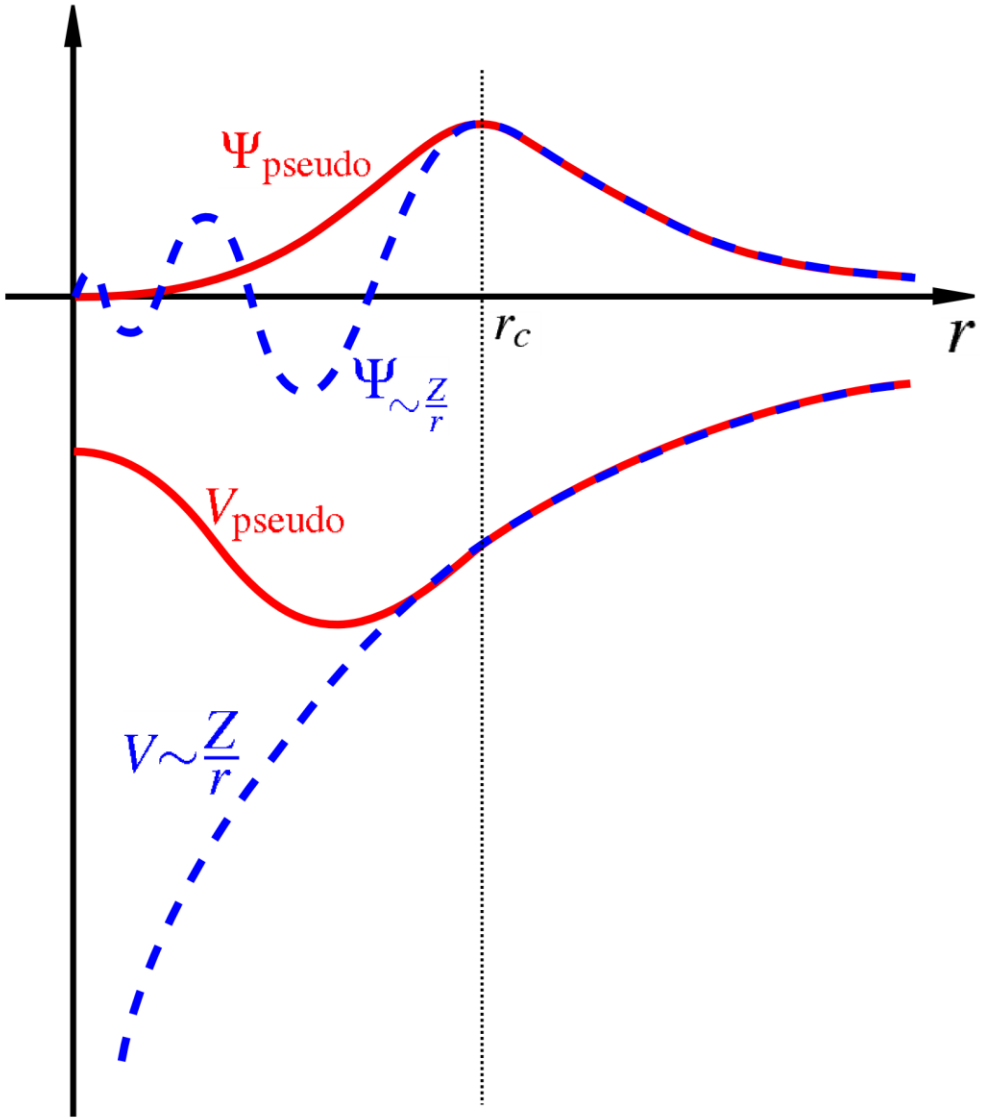
- Inclusion of core orbitals
  → corrects to valence and conduction bands near nuclei
  → *(all–electron effects)*
- EXCEED-DM adds core electrons after pseudopotential calculation
  → all–electron *reconstruction*
- New tool:
  ab-initio calculation including core orbitals

  'Quantum Chemistry Dark (QCDark)'*

  **Aman Singal*, Cheng Zhen (to appear)*



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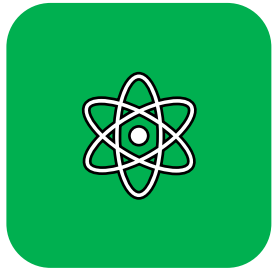

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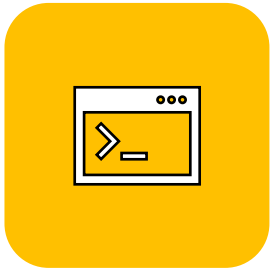

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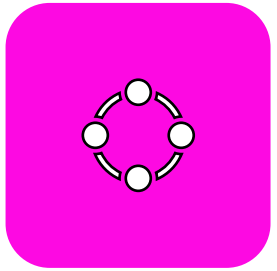
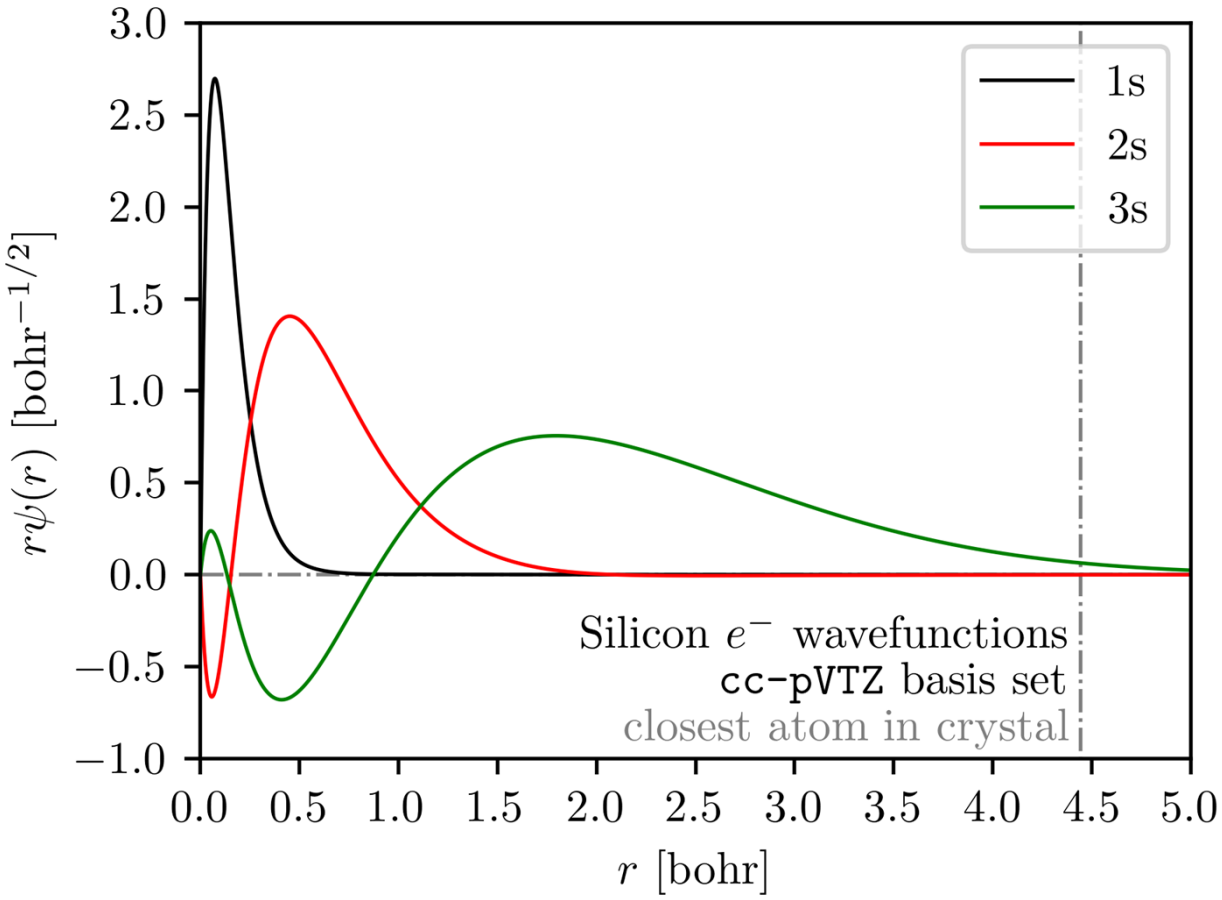


EFFECTS OF INCLUDING CORE ORBITALS

QUANTUM CHEMISTRY DARK (QCDARK)

Quantum Chemistry Dark, *QCDark*

- Based off PySCF –
  - Uses real space basis functions instead of plane waves
  - Wavefunctions are linear combinations of atomic orbitals
- QCDark to soon be available on GitHub!



PySCF: Sun (1412.0649); Sun et al. (1701.08223); Sun et al. (2002.12531)

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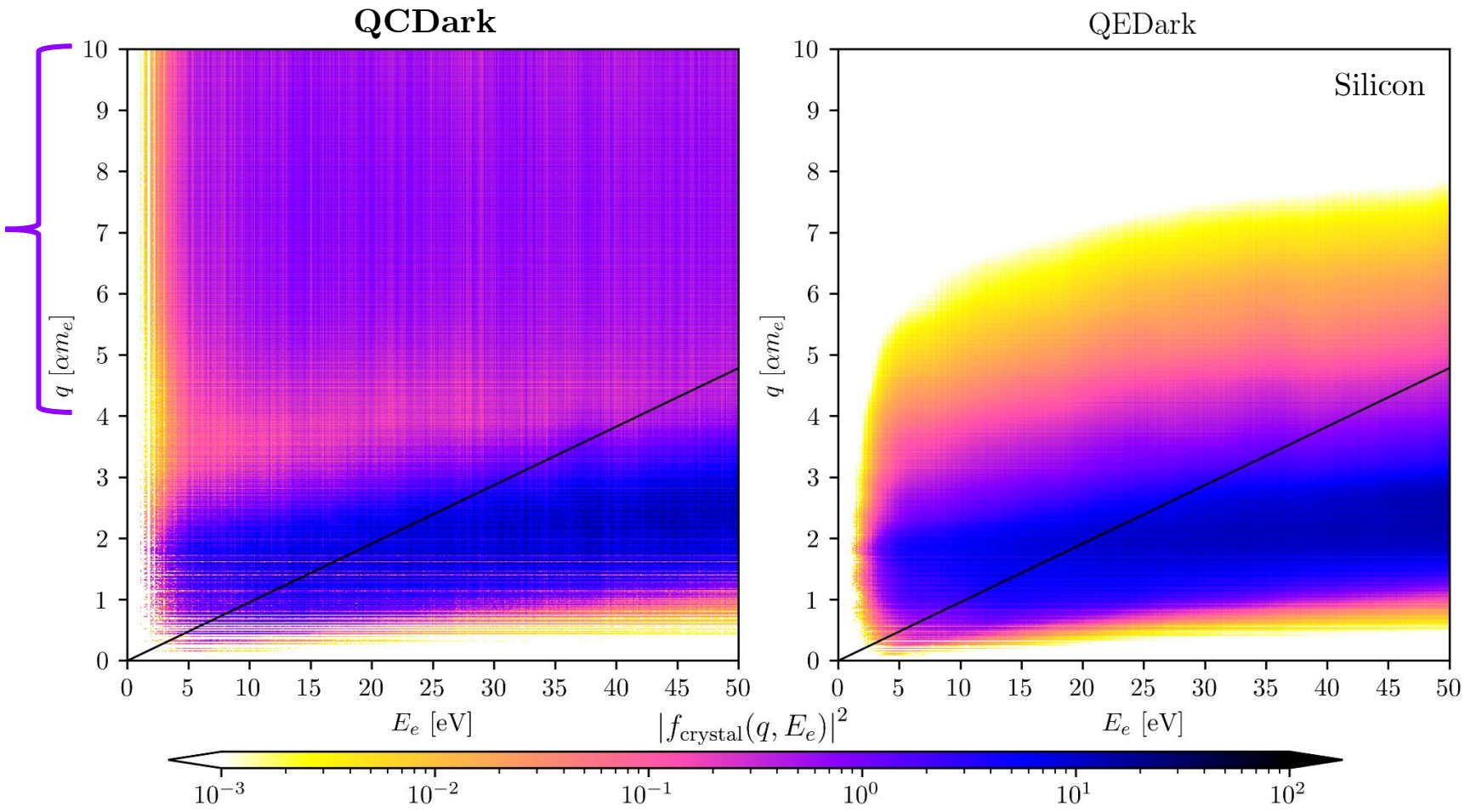
All–electron effects in the crystal form factor

Introduction of high momentum transfer modes!



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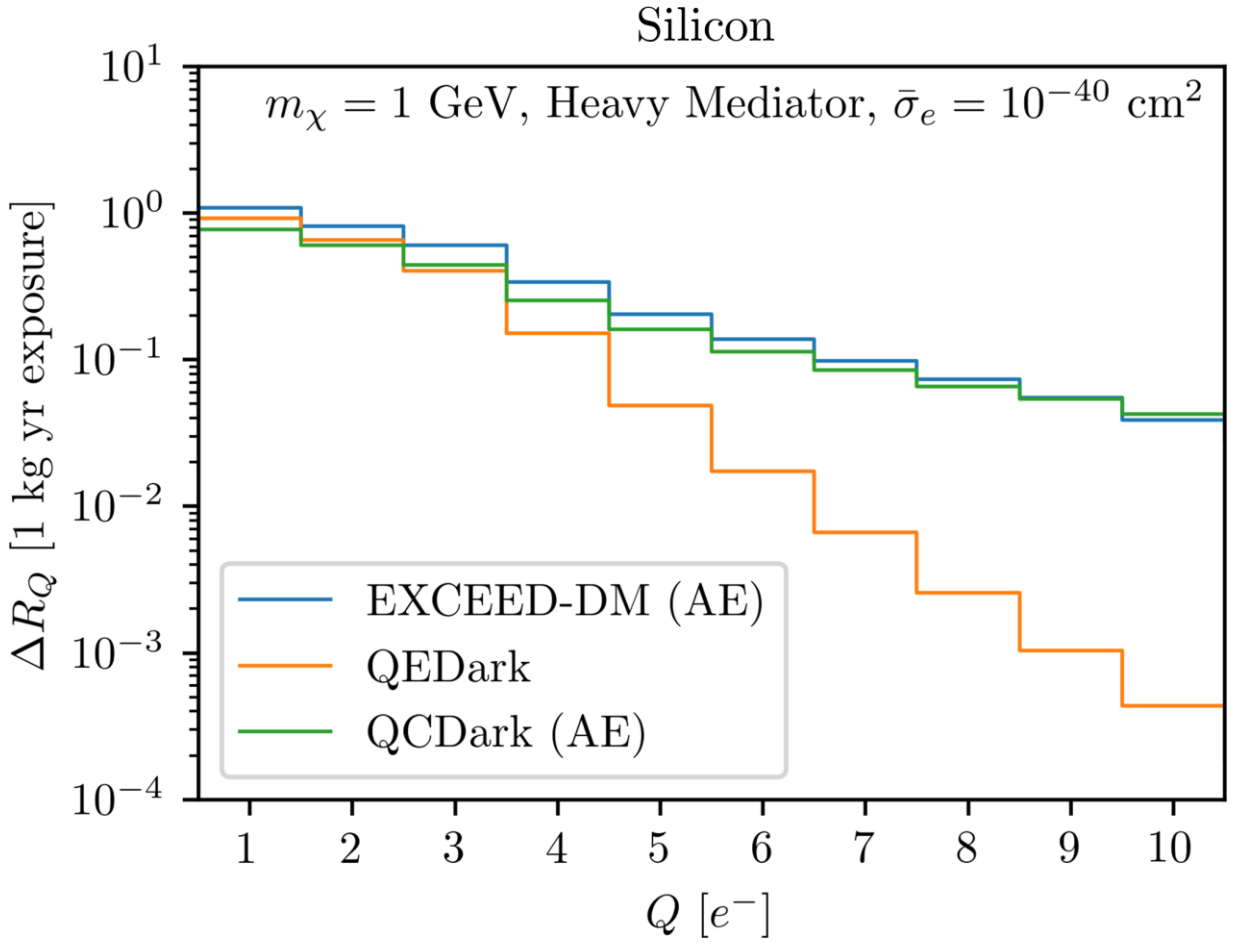
All–electron effects (AE) increases scattering rates

- All–electron allows correct modelling of dark matter–electron scatterings with large momentum transfer, *q*
- Large (order of magnitude) enhancement of rates for larger dark matter mass at high ΔE



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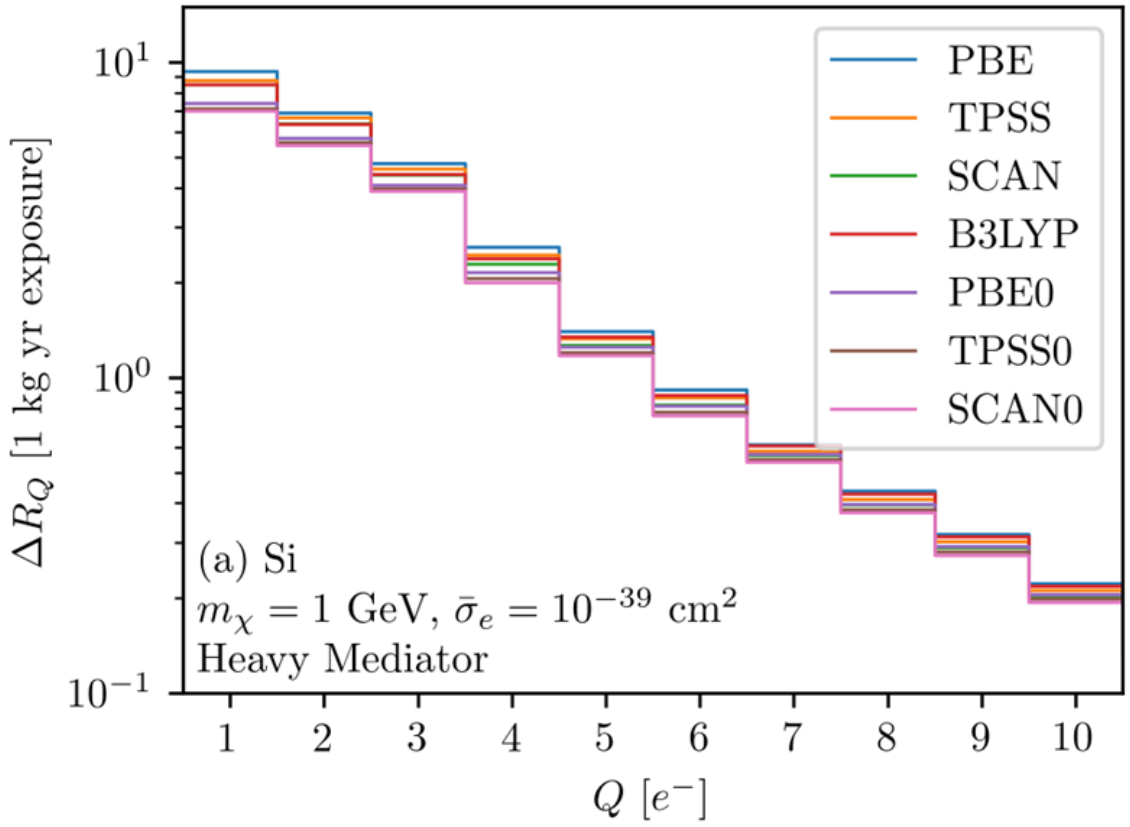
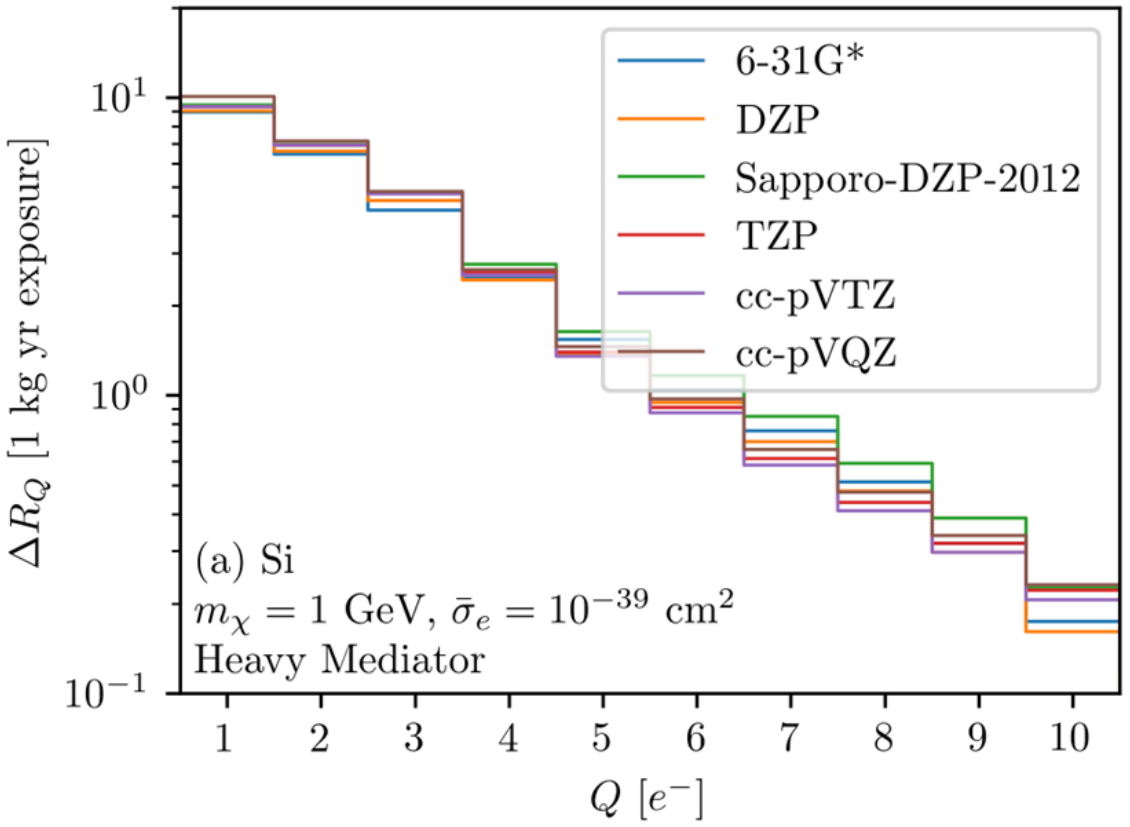
Theory uncertainties in dark matter–electron scattering rates

Exchange-correlation functional



Choice of basis set



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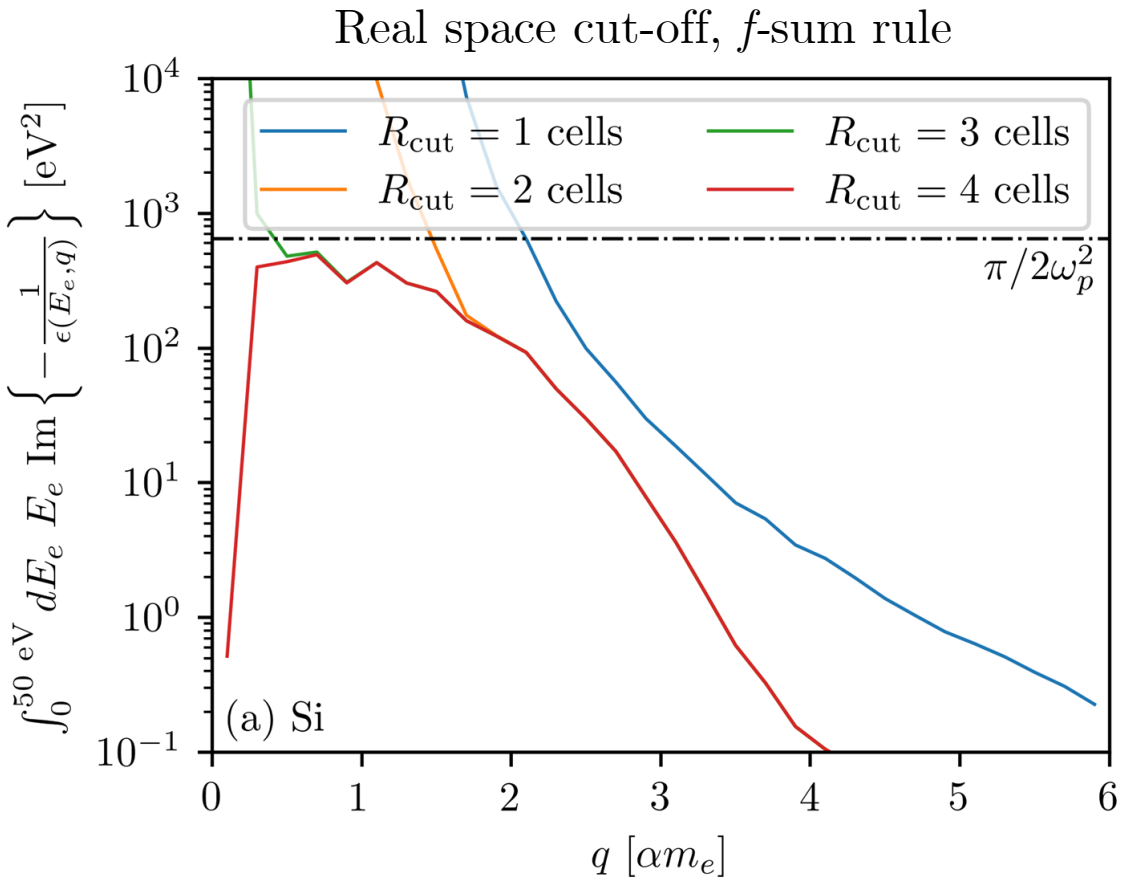

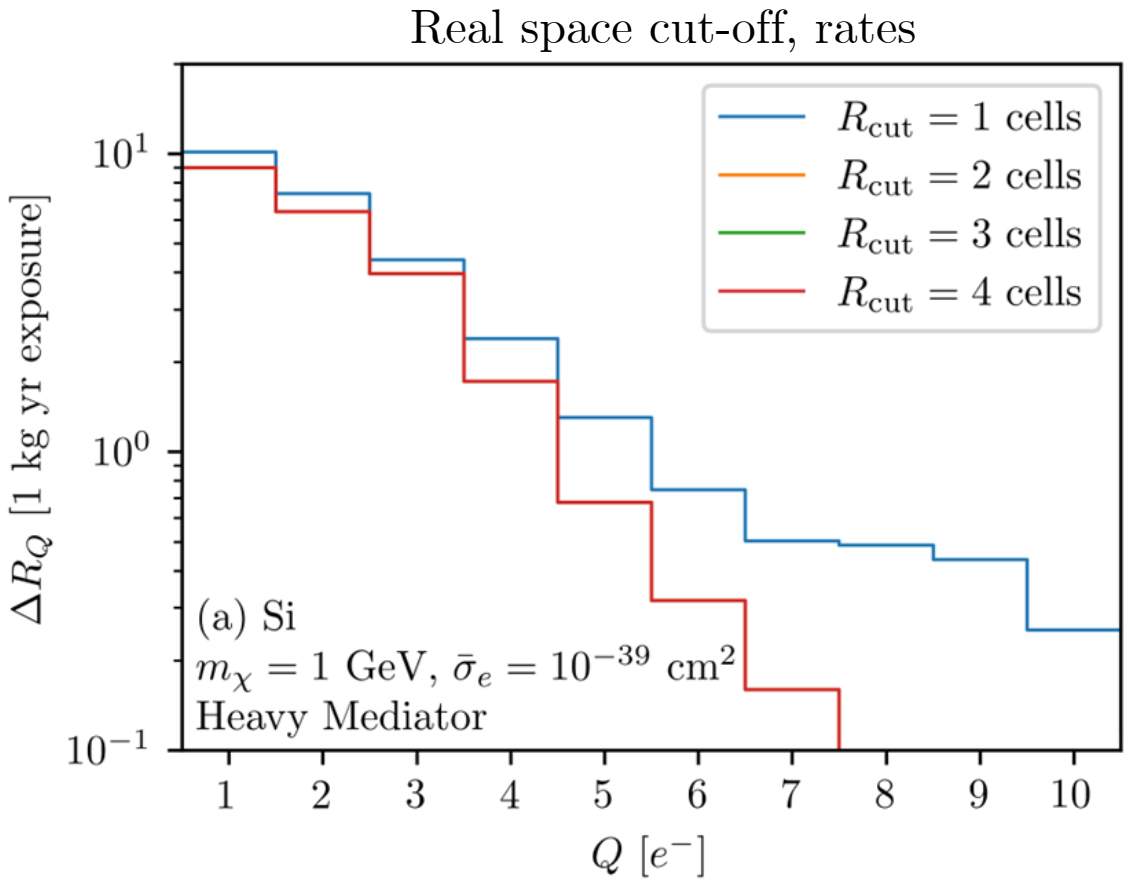

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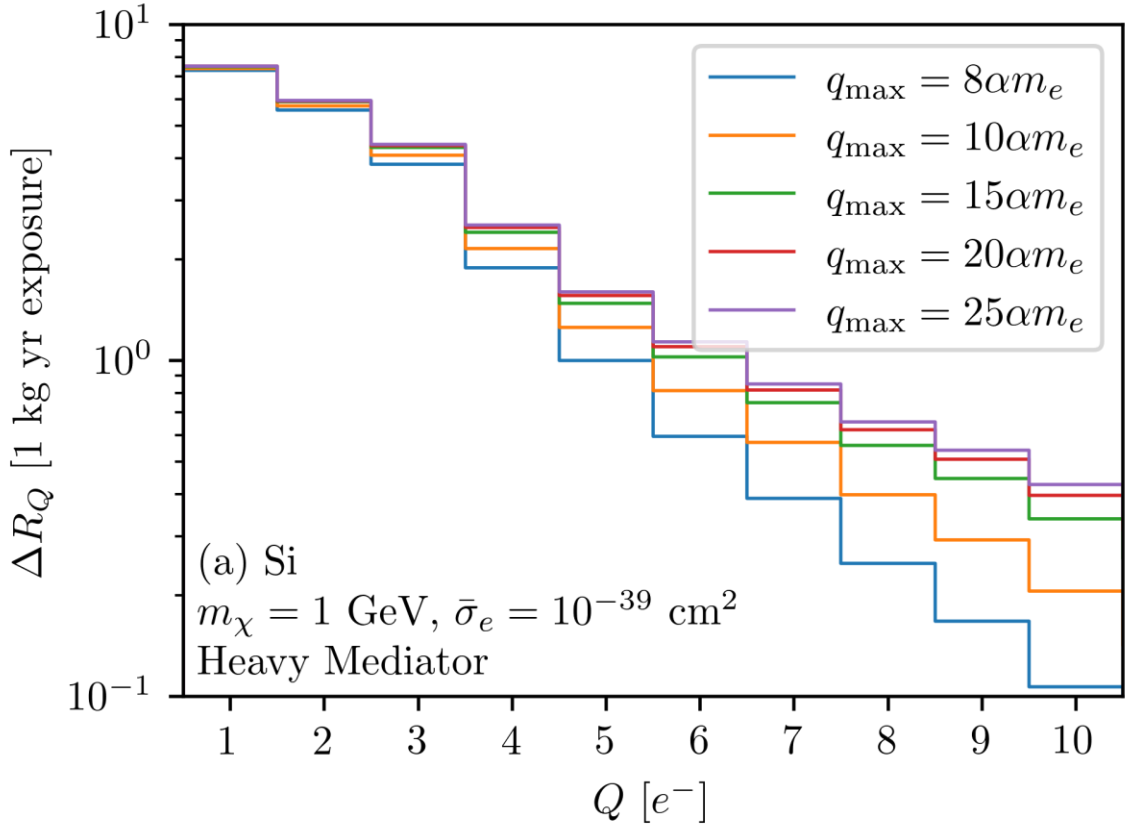
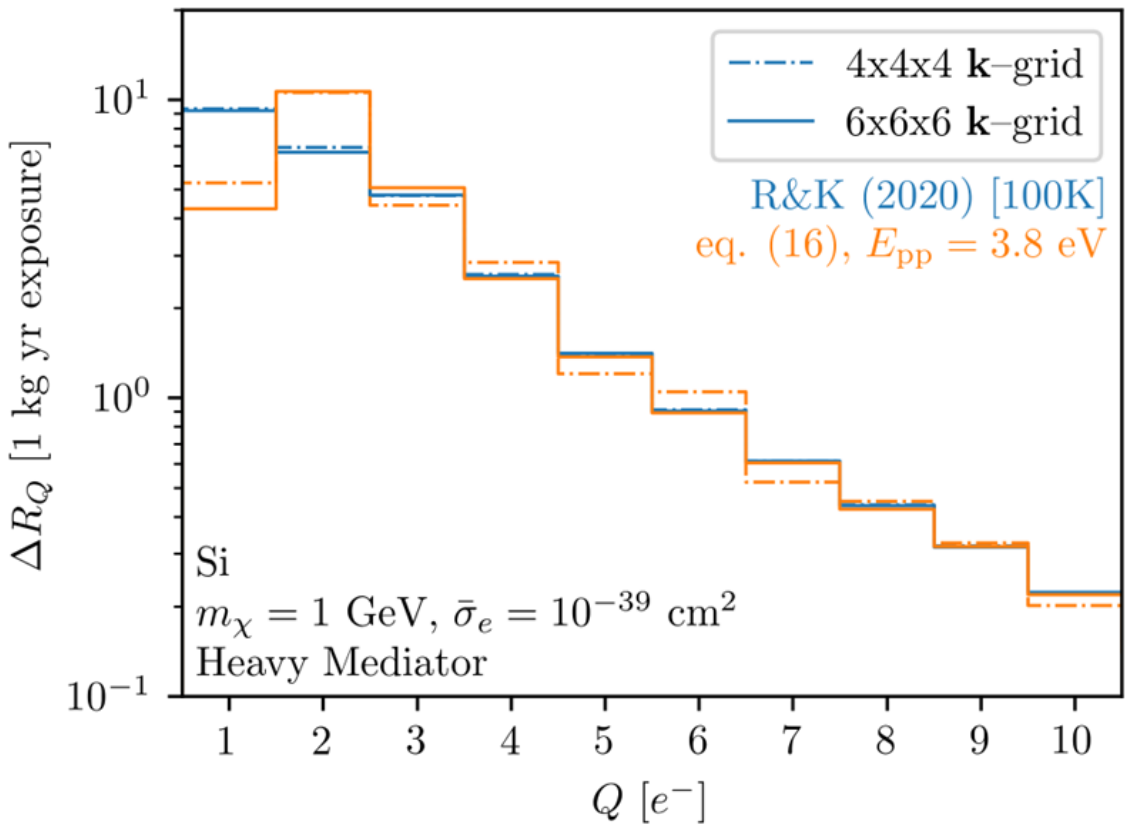
Theory uncertainties in dark matter–electron scattering rates

Maximum momentum transfer modelled



Secondary ionization and grid in 1st BZ



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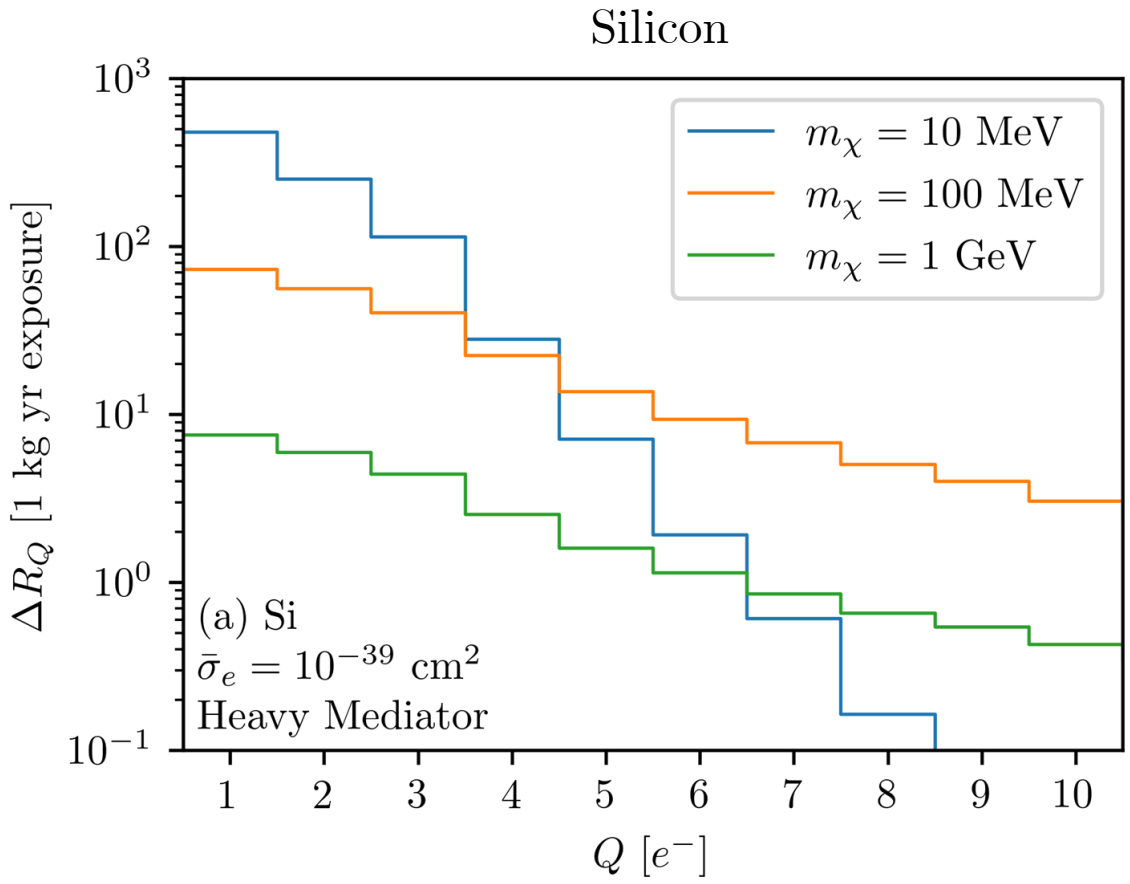
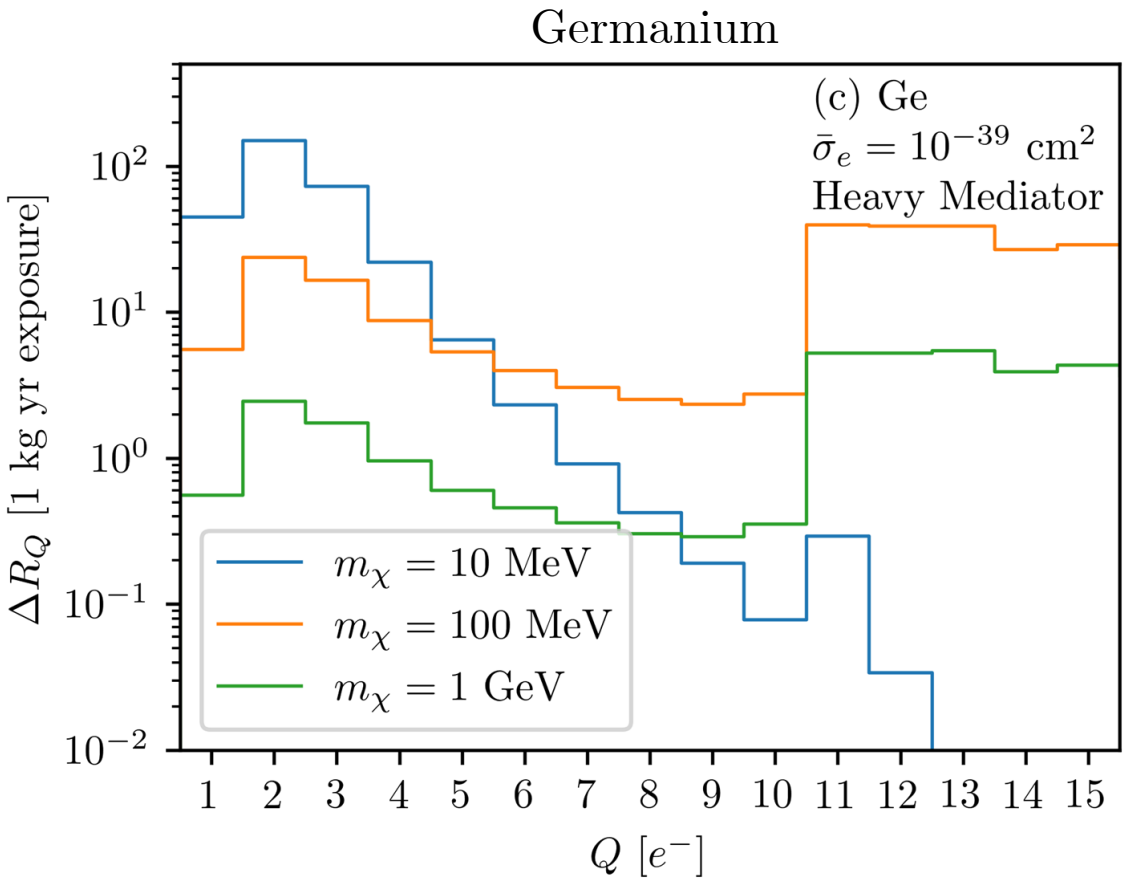
R&K: Ramanathan & Kurinsky (2004.10709)

Rate calculation with QCDark





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Conclusion

- Large ongoing experimental effort in sub-GeV dark matter direct detection –
  dark matter-electron scattering experiments (SENSEI, DAMIC, SuperCDMS, …)
- Need to understand theory better –
  - Inclusion of core orbitals increases expected dark matter–electron scattering rates at high energy transfer ΔE
  - Also need to properly analyze theory uncertainties associated with these rates
- Quantum Chemistry Dark (QCDark) does a fully *ab-initio* calculation including core orbitals using PySCF as base for density functional theory.
  - We perform a systematic analysis of theory uncertainties in dark matter–electron scattering rates in Si and Ge.

QCDark to be made publically available on GitHub upon submission of paper to arXiv!

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Thank You!

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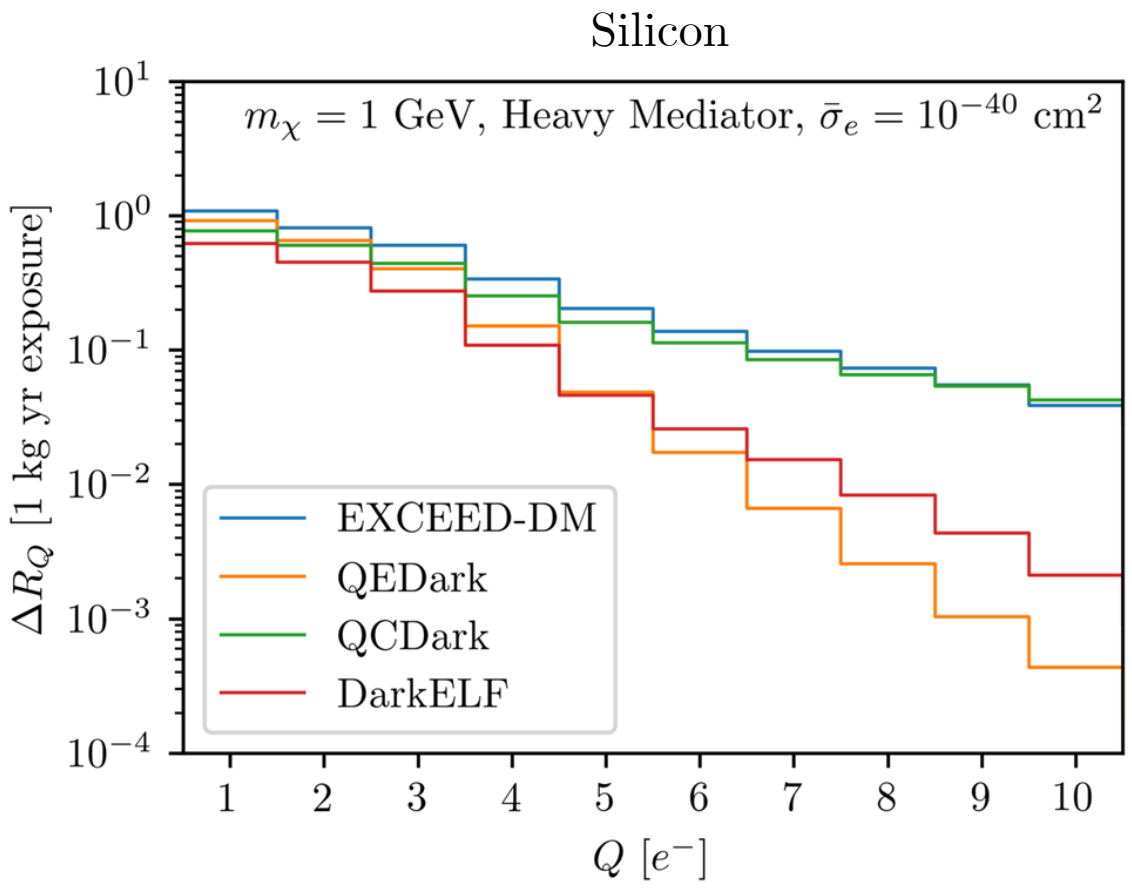
Comparison of available codes

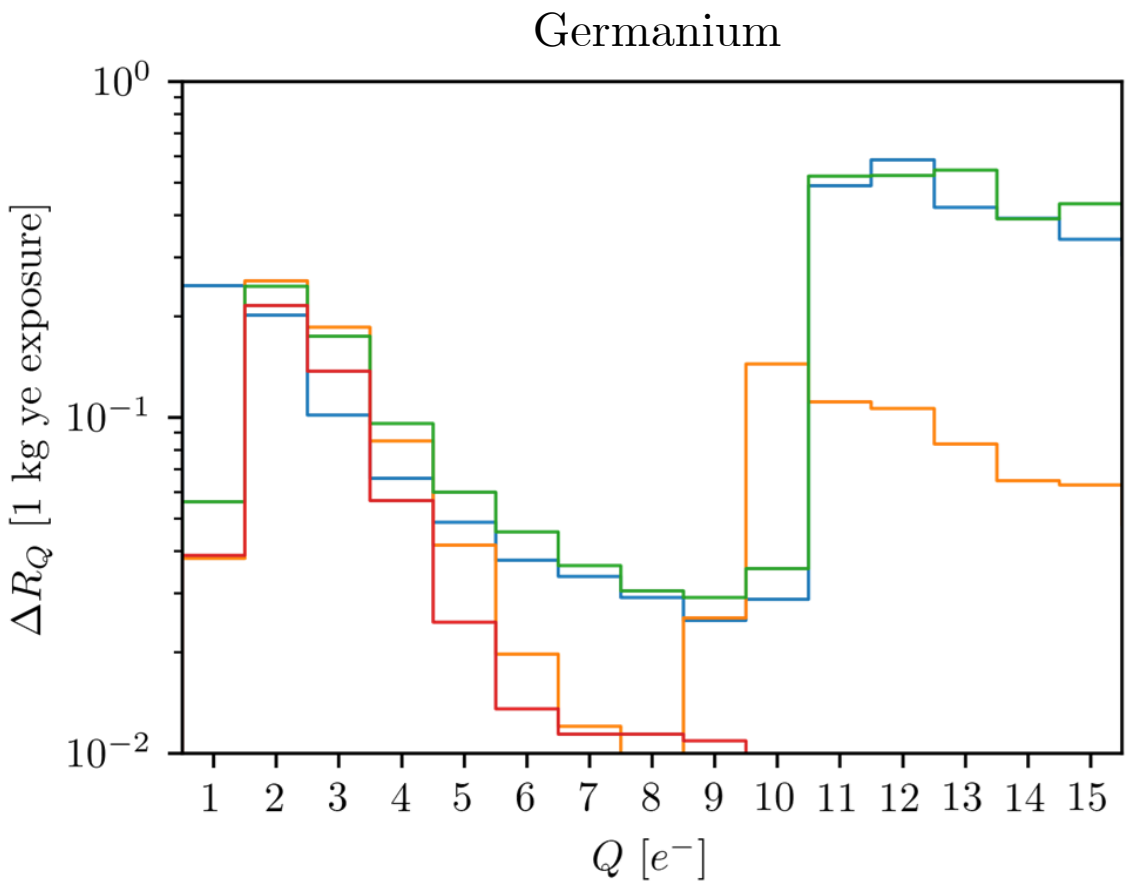
Code	**Calculation Type**	**Screening**	**All-electron effects**
QEDark	CFF[1]	None[2]	None
DarkELF	Dielectric function[3]	Numerical	None
EXCEED-DM	CFF + Dielectric	Numerical + Analytical	Reconstruction
QCDark	CFF	Analytical	*Ab-initio*

1. Refers to crystal form factor.
2. It is trivial to add analytical screening to QEDark, and all plots in this presentation included it.
3. DarkELF consists of precalculated look-up tables and does not offer computation for new prospective materials.

QCDark: Cyrus Dreyer, Rouven Essig, Marivi Fernandez-Serra, AS, Cheng Zhen (to appear)
QEDark: Essig, Fernandez-Serra, Mardon, Soto, Yu (1509.01598)
DarkELF: Knapen, Kozaczuk, Lin (2101.08275, 2104.12786); see also Hochberg, Kahn, Kurinsky, Lehmann, Yu, Berggren (2101.08263)
EXCEED-DM: Griffin, Inzani, Trickle, Zhang, Zurek (2105.09567), Trickle (2210.14917)

Comparison of available codes





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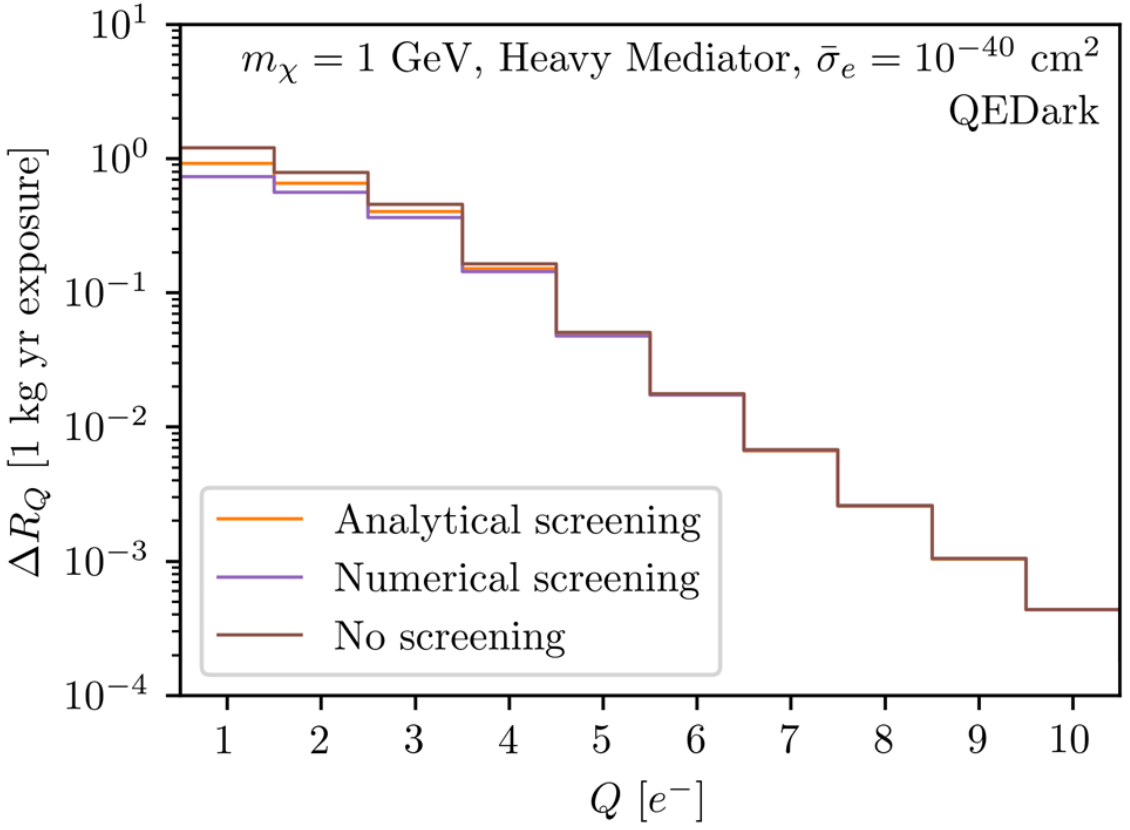
Screening

- DarkELF (2021) showed electrostatic screening effects are important at low charge ionization.

$$\left|f_{\text{crystal}}(q,\Delta E)\right|^2 \rightarrow \frac{\left|f_{\text{crystal}}(q,\Delta E)\right|^2}{\left|\epsilon(q,\Delta E)\right|^2}$$



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Screening

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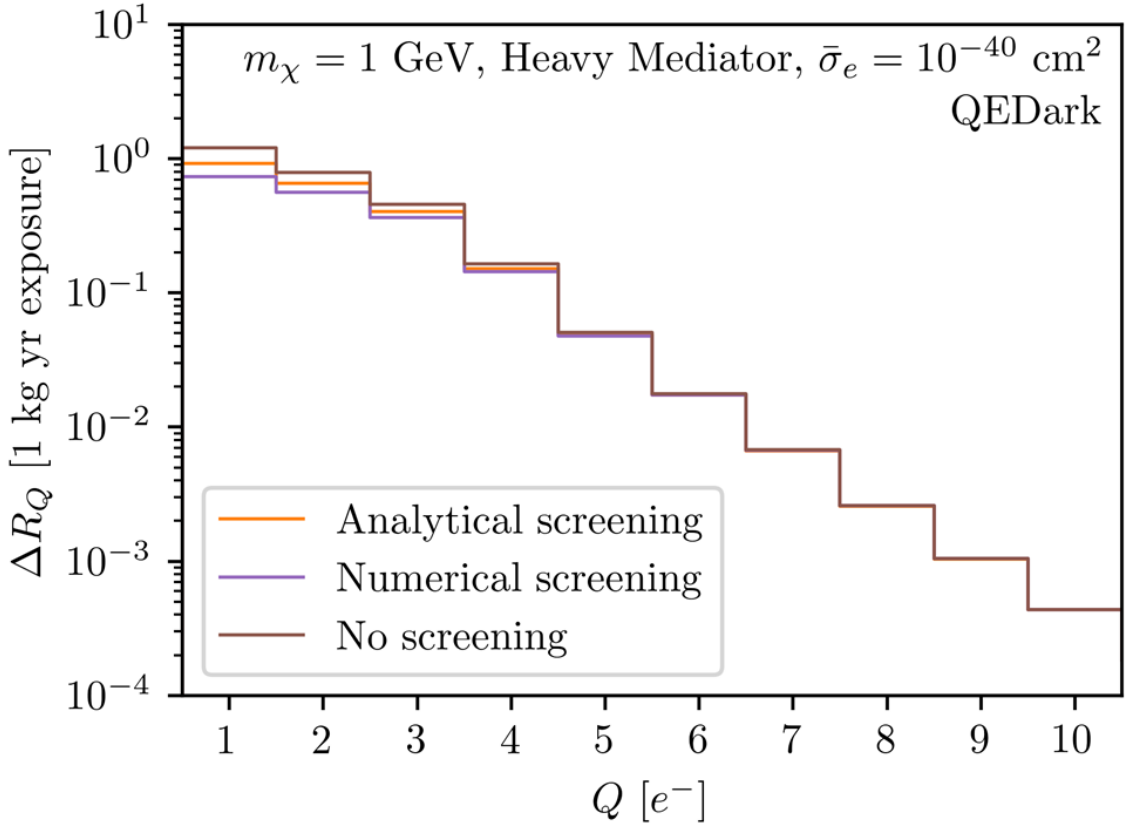
$$|f_{\text{crystal}}(q, \Delta E)|^2 \rightarrow \frac{|f_{\text{crystal}}(q, \Delta E)|^2}{|\epsilon(q, \Delta E)|^2}$$

We call this the dielectric function!



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