中国暗物质实验
China Dark matter EXperiment

四川大學

Investigating Ultra-Low Energy Ionization Yield from Nuclear Recoils in Semiconductor Detectors via Molecular Dynamics Simulations

Speaker: Chang-Hao Fang

On behalf of CDEX-SCU group

TAUP XICHANG

Email: fangch@stu.scu.edu.cn

- **Low-energy Nuclear Recoil and Ionization Quenching**
- Molecular Dynamic Methods
- Results and Roadmap for Silicon and Germanium
- Impact on Dark Matter Searches
- Summary and Future Prospects

Low-energy Nuclear Recoil Channel in Particle Physics

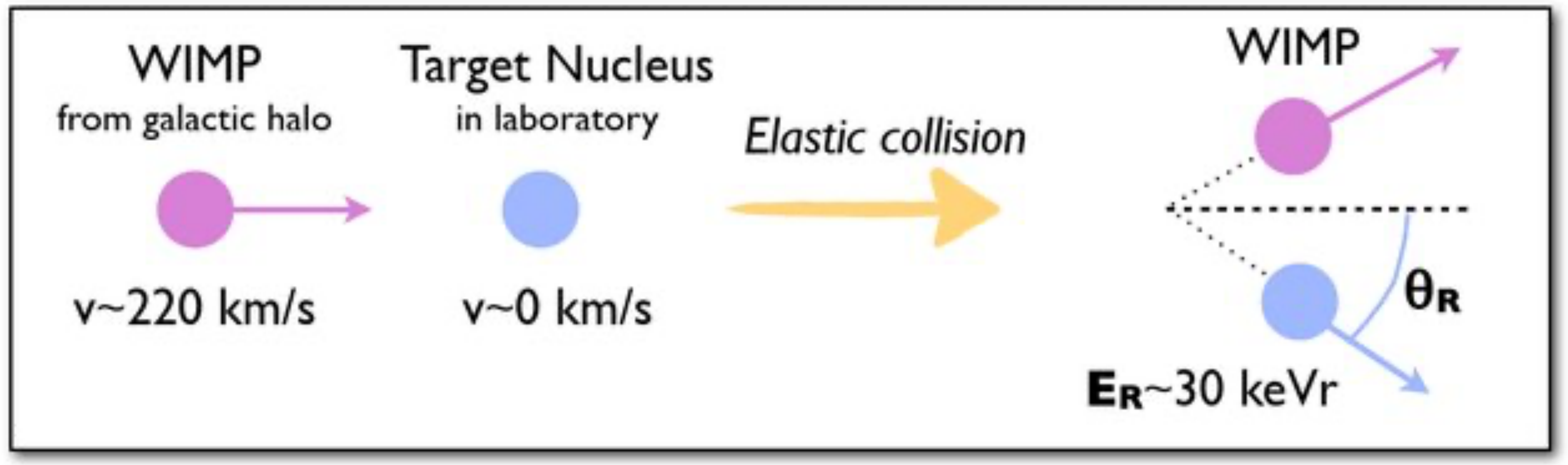
Si

SUPER CDMS

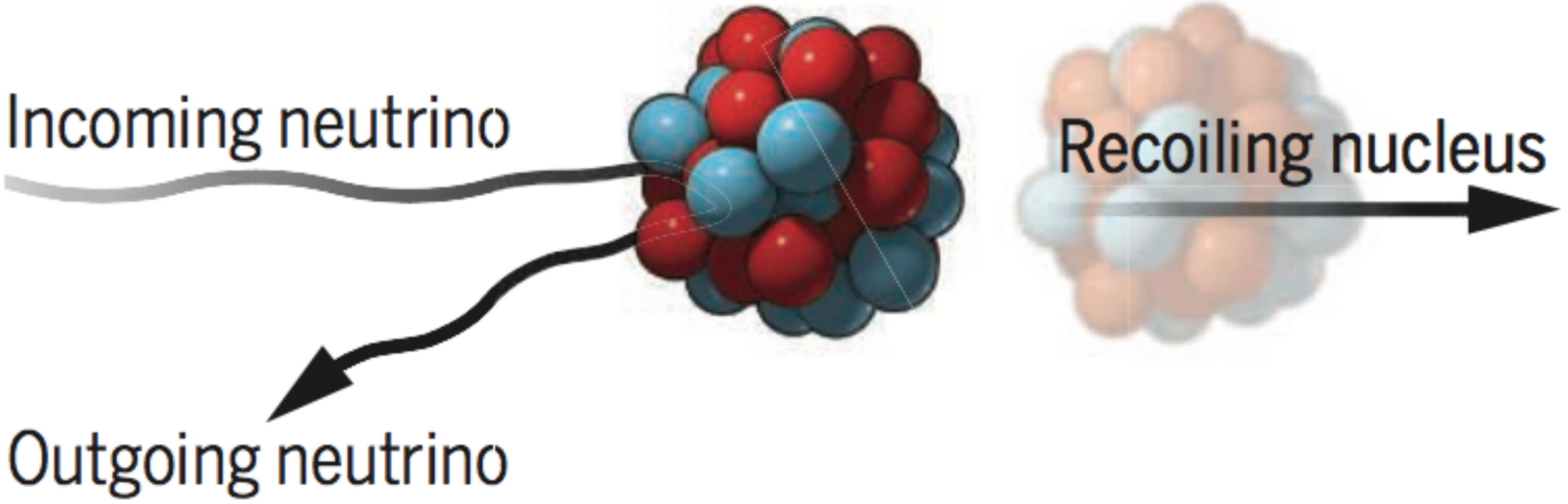
CO.νNie
COHERENT NEUTRINO NUCLEUS INTERACTION EXPERIMENT

DAMIC-M

Etc.



χ-N scattering



Coherent Elastic neutrino Nuclear Scattering (CEvNS)

Ge

中国暗物质实验
China Dark matter EXperiment

臺灣微中子實驗
TEXONO
Taiwan EXperiment On NeutrinO

CONUS

Etc.

Ionization Quenching on Low-energy Nuclear Recoil

Ionization Quenching Factor (QF) (< 1)

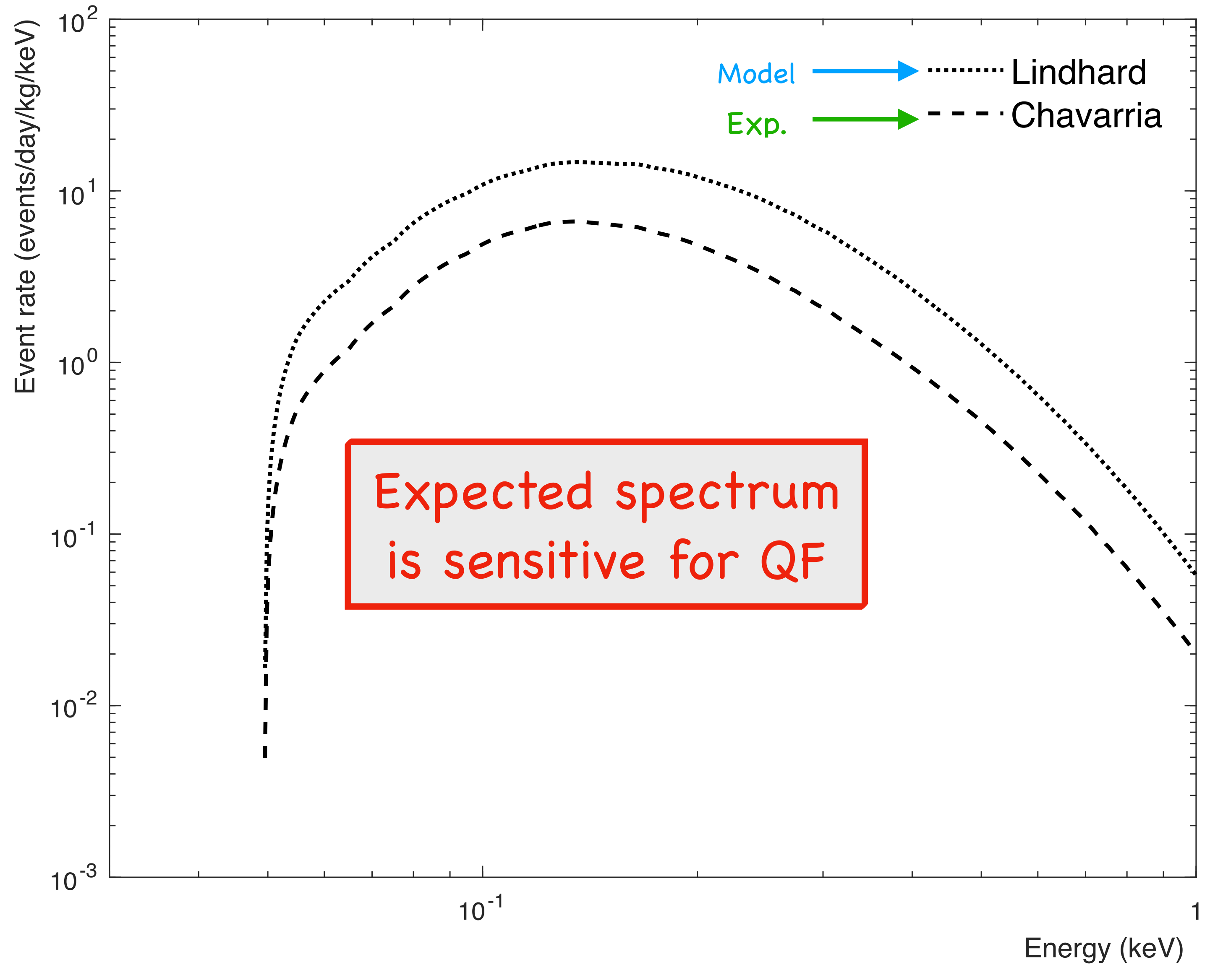
$$E_{ee} = Q \times E_{nr}$$

Measured Energy — Nucl. Recoil Energy

Detector Ionization Response

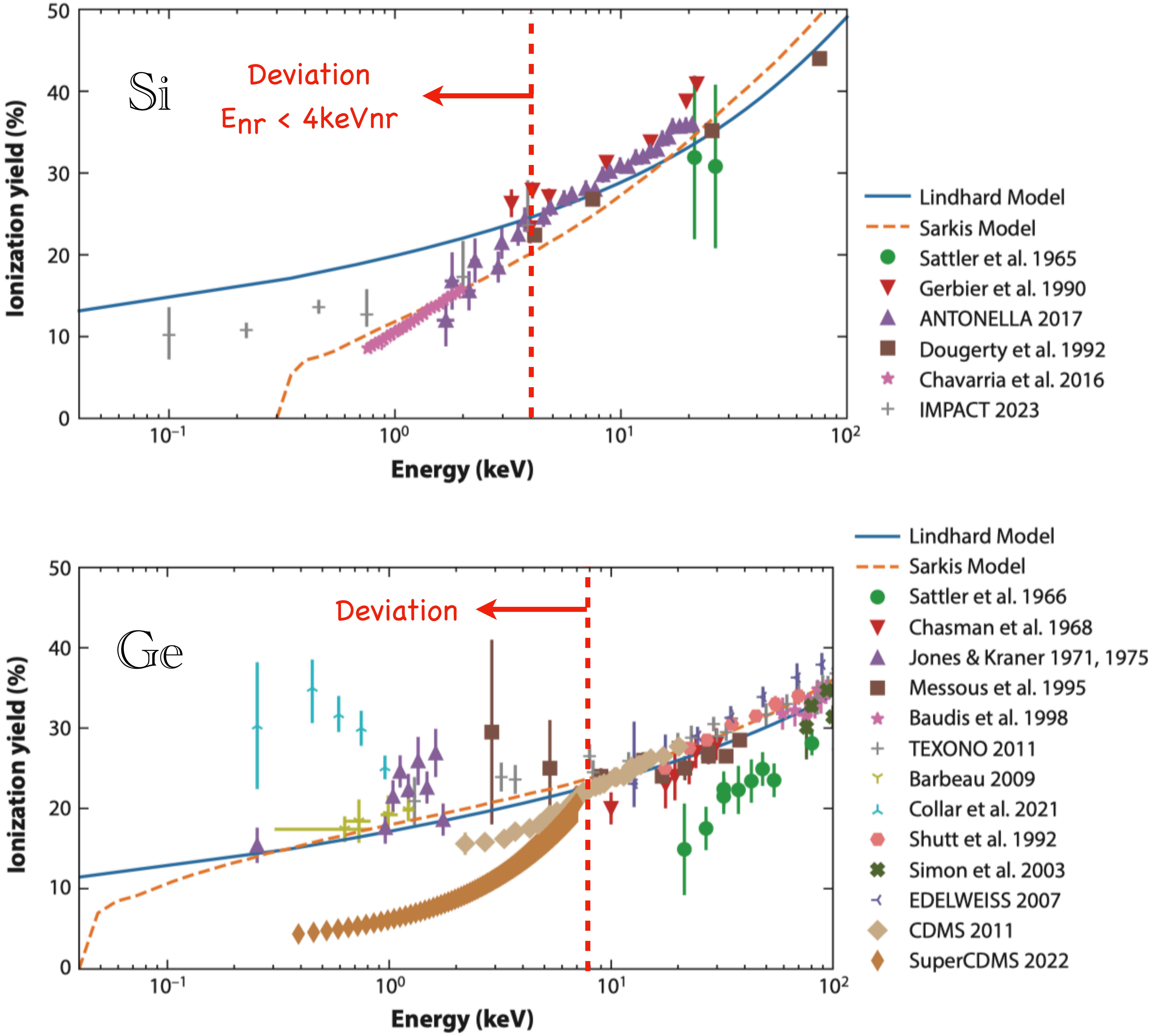
$$\frac{dR}{dE_{ee}} = \frac{dR}{dE_{nr}} \frac{1}{Q}\left(1 + \frac{E_{nr}}{Q}\frac{dQ}{E_{nr}}\right)^{-1}$$

Exp. Spectrum — Theoretical Spectrum



CEvNS's expected event rate dependence on QF. [CONNIE2019]

- QFs are unavoidable detector response for ionization/scintillation detection.
- A considerable source of uncertainty for physical results interpretation.

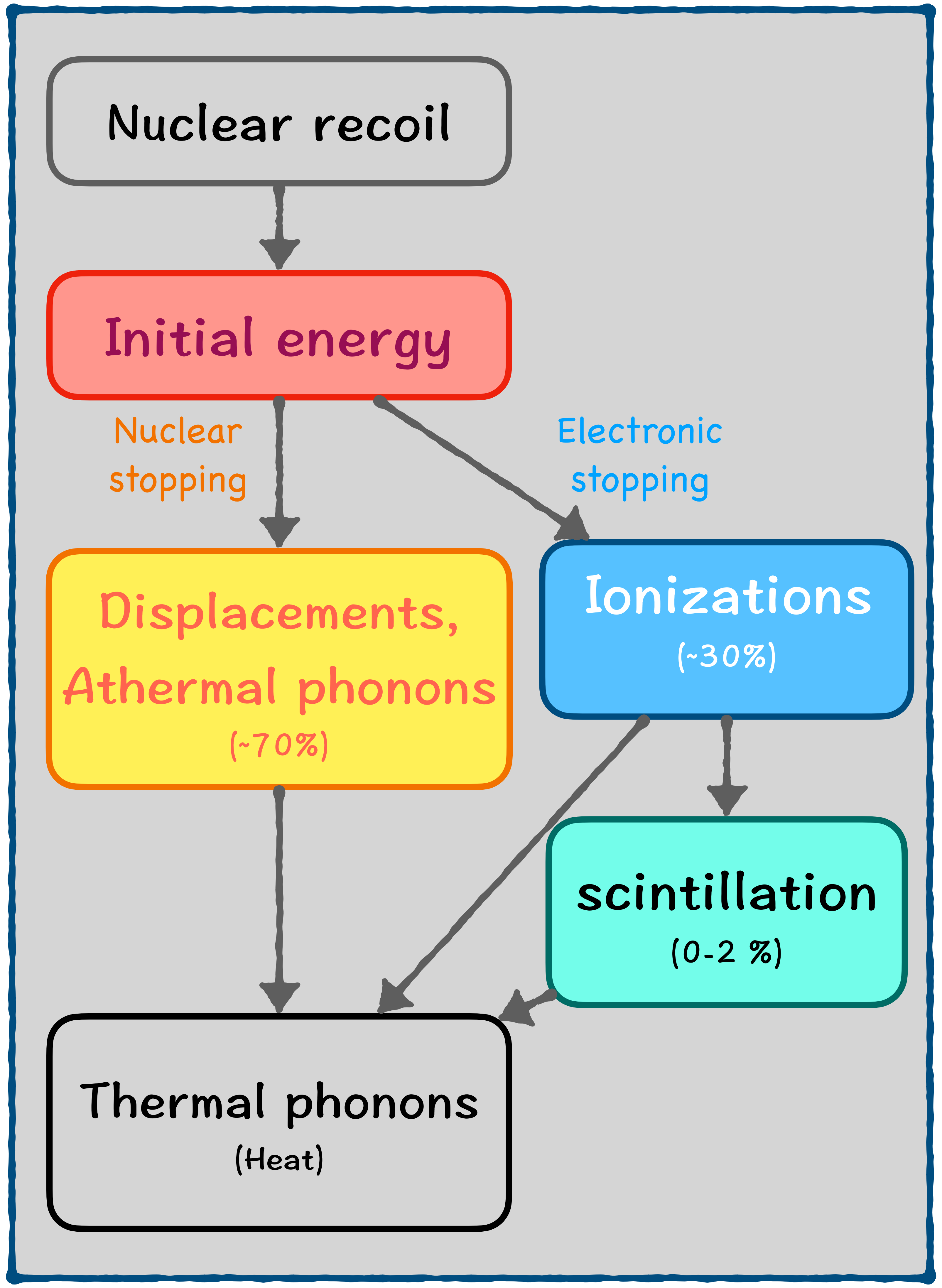


Ionization yields of Si (top) and Ge (bottom) measurements [1].

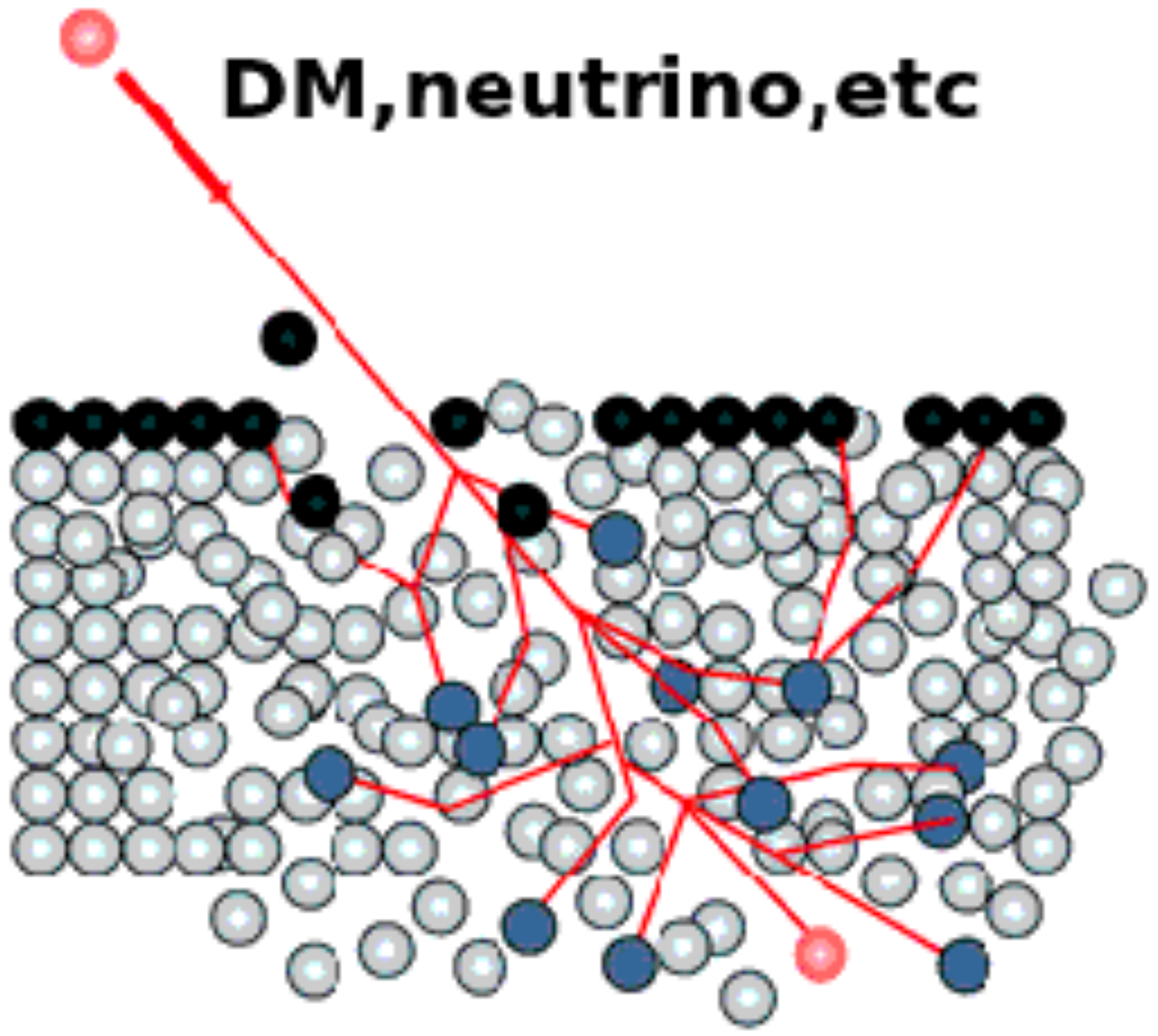
[1] J. Xu, P. S. Barbeau, Z. Hong, Detection and Calibration of Low-Energy Nuclear Recoils for Dark Matter and Neutrino Scattering Experiments. *Annu. Rev. Nucl. Part. Sci.* **73**, 95–121 (2023).

- Low-energy Nuclear Recoil and Ionization Quenching
- **Molecular Dynamic Methods**
- Results and Roadmap for Silicon and Germanium
- Impact on Dark Matter Searches
- Summary and Future Prospects

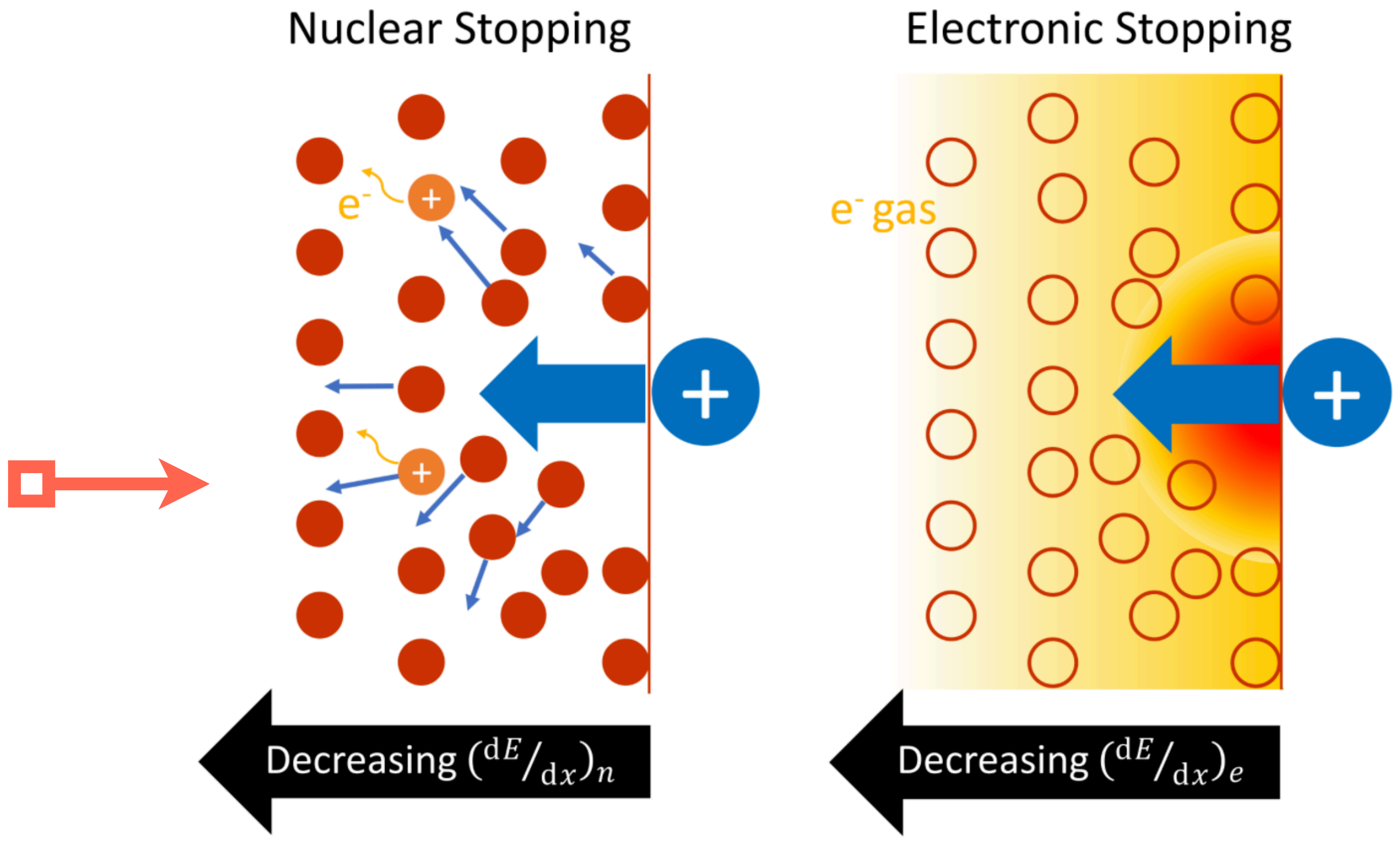
Picture of Ionization Quenching



Signals from recoils



Stopping process of nuclear recoil event



Nuclear and electronic stopping

- Competition of energy loss process: Nucl. vs. Elec.
- Picture of quenching: Nucl. Recoil energy -> Displacements, Vibrations + Ionization (visible energy).

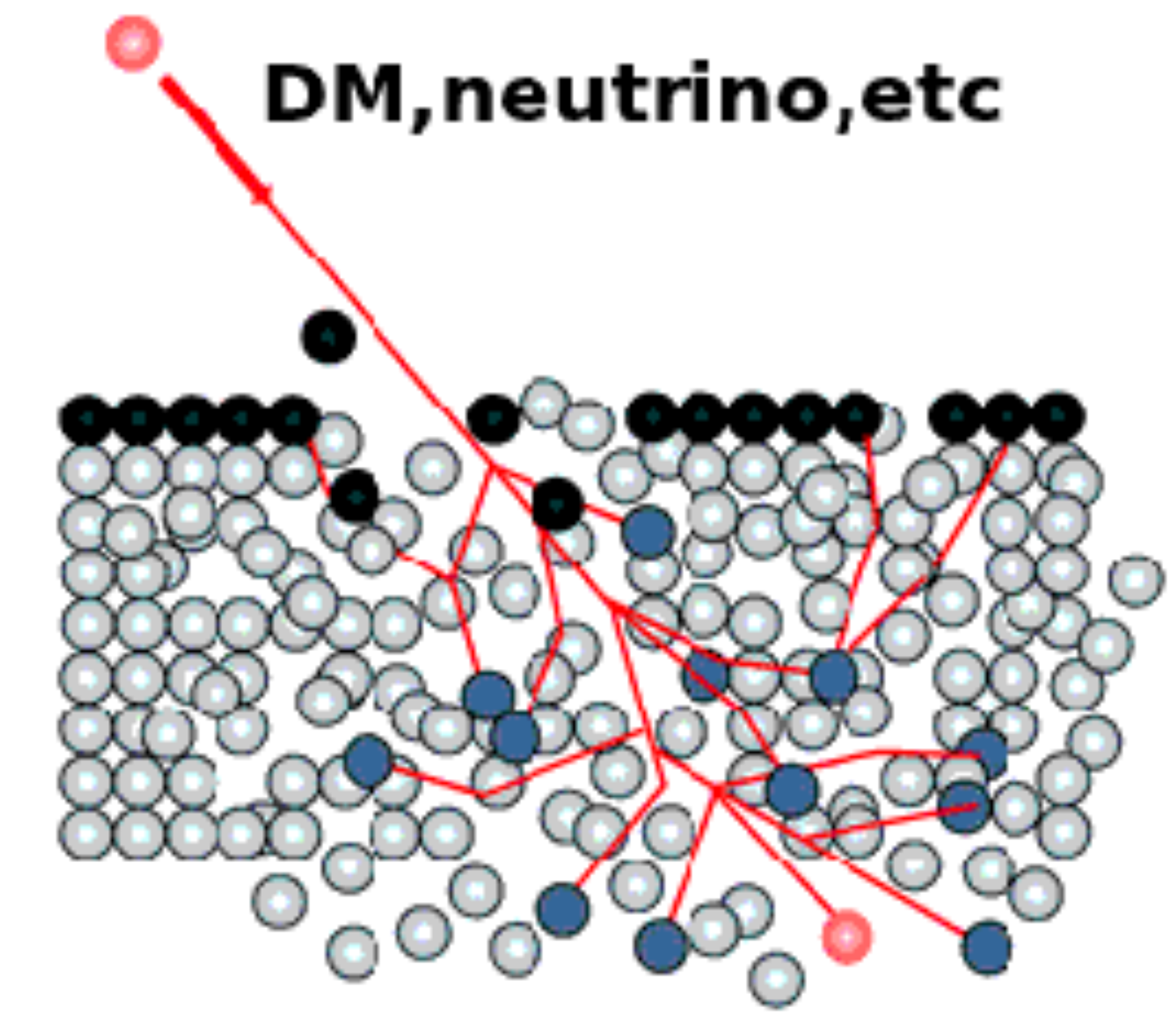
Molecular Dynamics Approach

$$Q = E_{ee}/E_{nr}$$

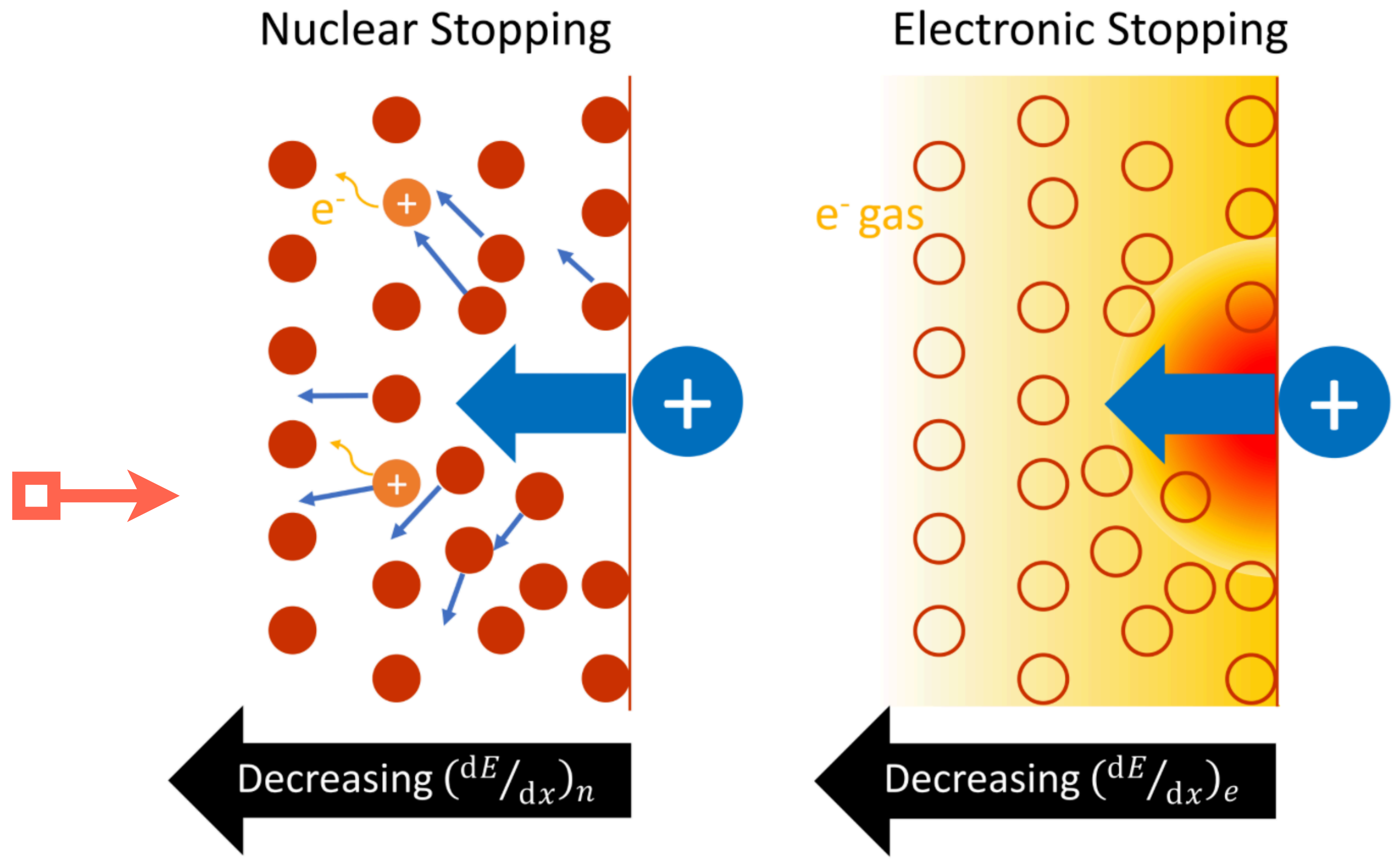
Lindhard's (five) approximations

- I. Neglect contribution to atomic motion coming from electrons.
- II. **Neglect the binding energy, U = 0.**
- III. The energy transferred to ionized electrons is small compared to that transferred to recoiling ions.
- IV. Effects of electronic and atomic collisions can be treated separately.
- V. T_n is also small compared to the energy E.

Expected to be valid for sufficiently high energies.



Stopping process of nuclear recoil event

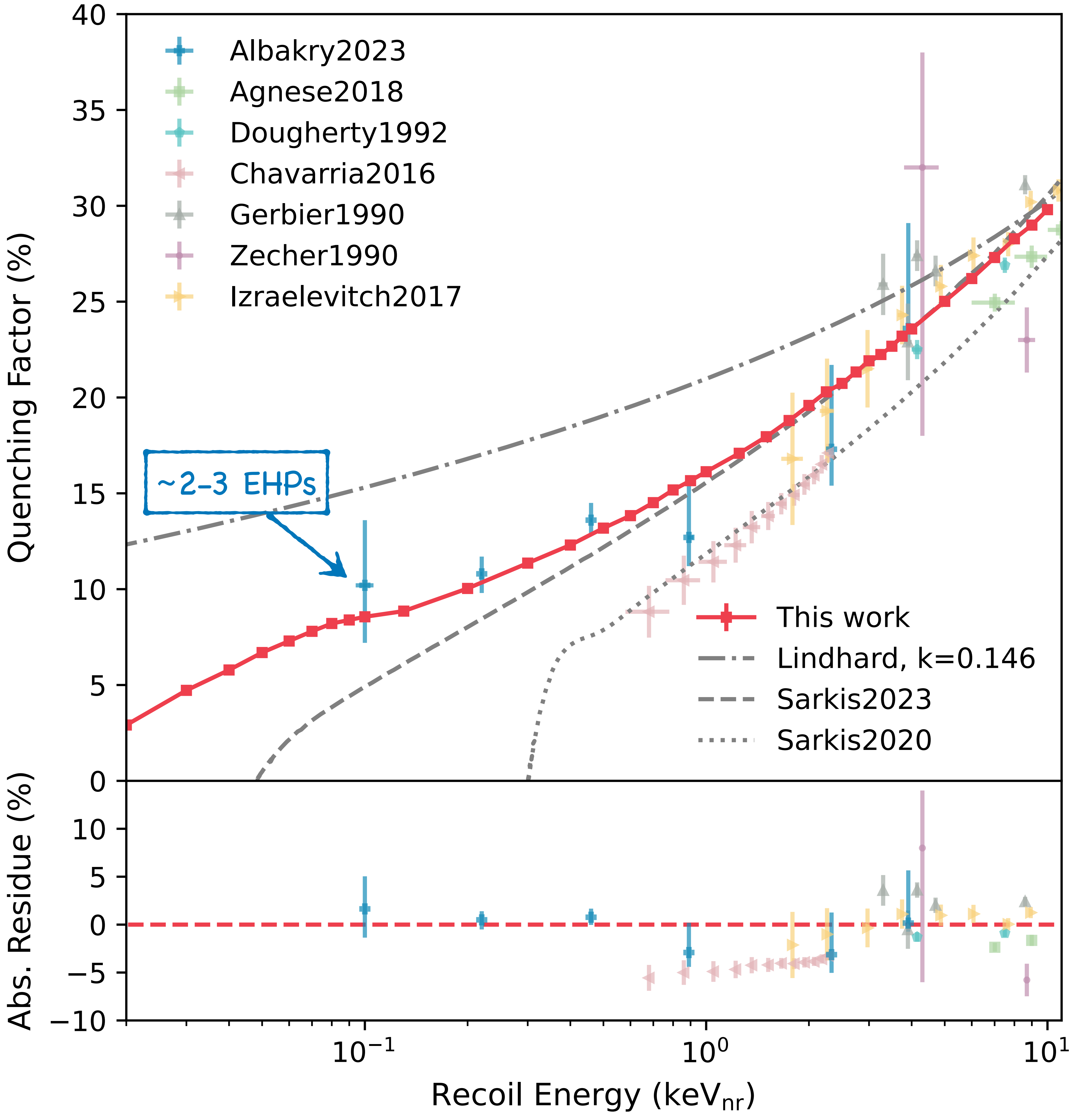


Nuclear and electronic stopping

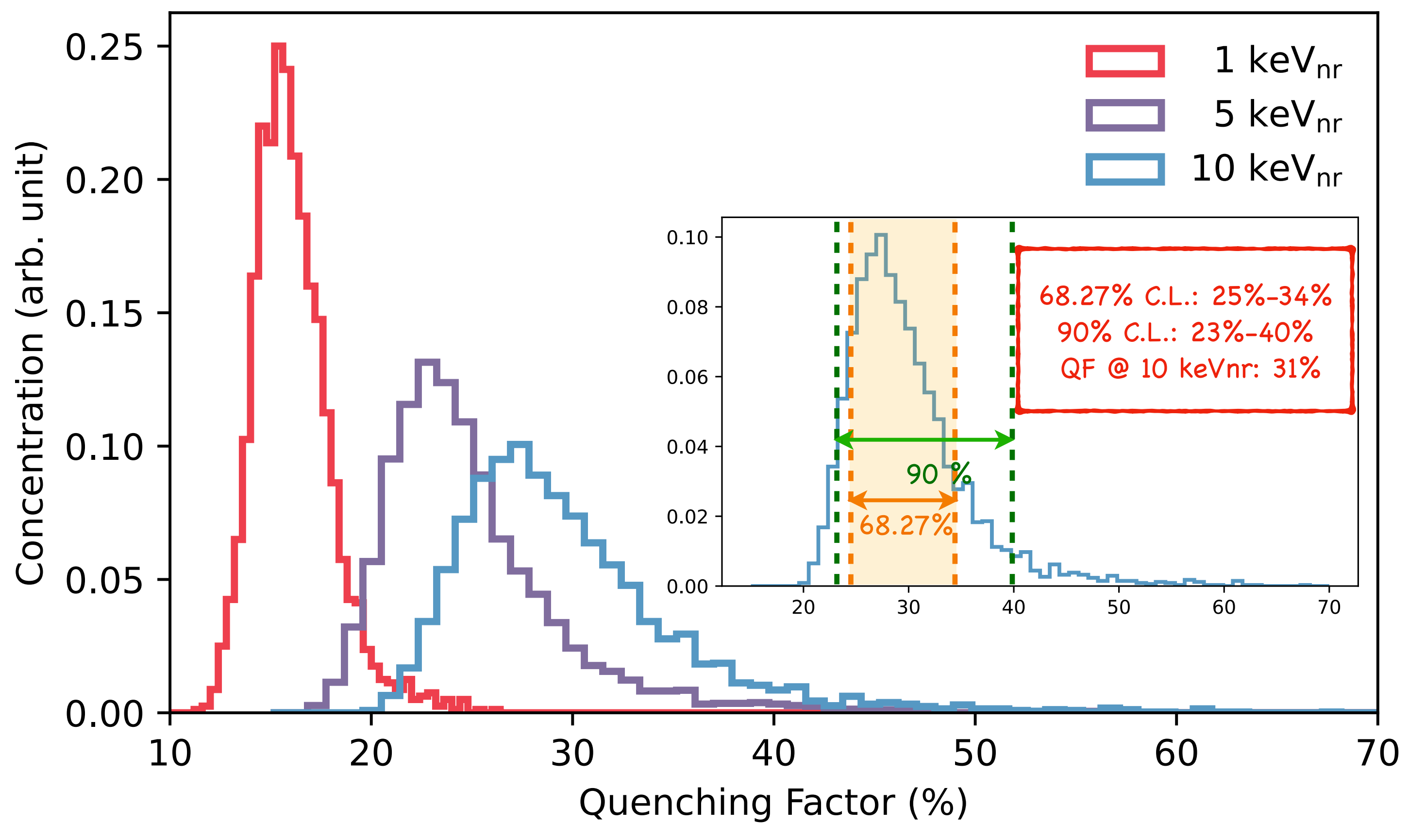
- Intuitively models energy allocation to ionization during nuclear recoil transport.
- Naturally incorporates highly anisotropic lattice binding and structure into atomic collision processes. (Beyond Lindhard model)

- Low-energy Nuclear Recoil and Ionization Quenching
- Molecular Dynamic Approach
- **Results and Roadmap for Silicon and Germanium**
- Impact on Dark Matter Searches
- Summary and Future Prospects

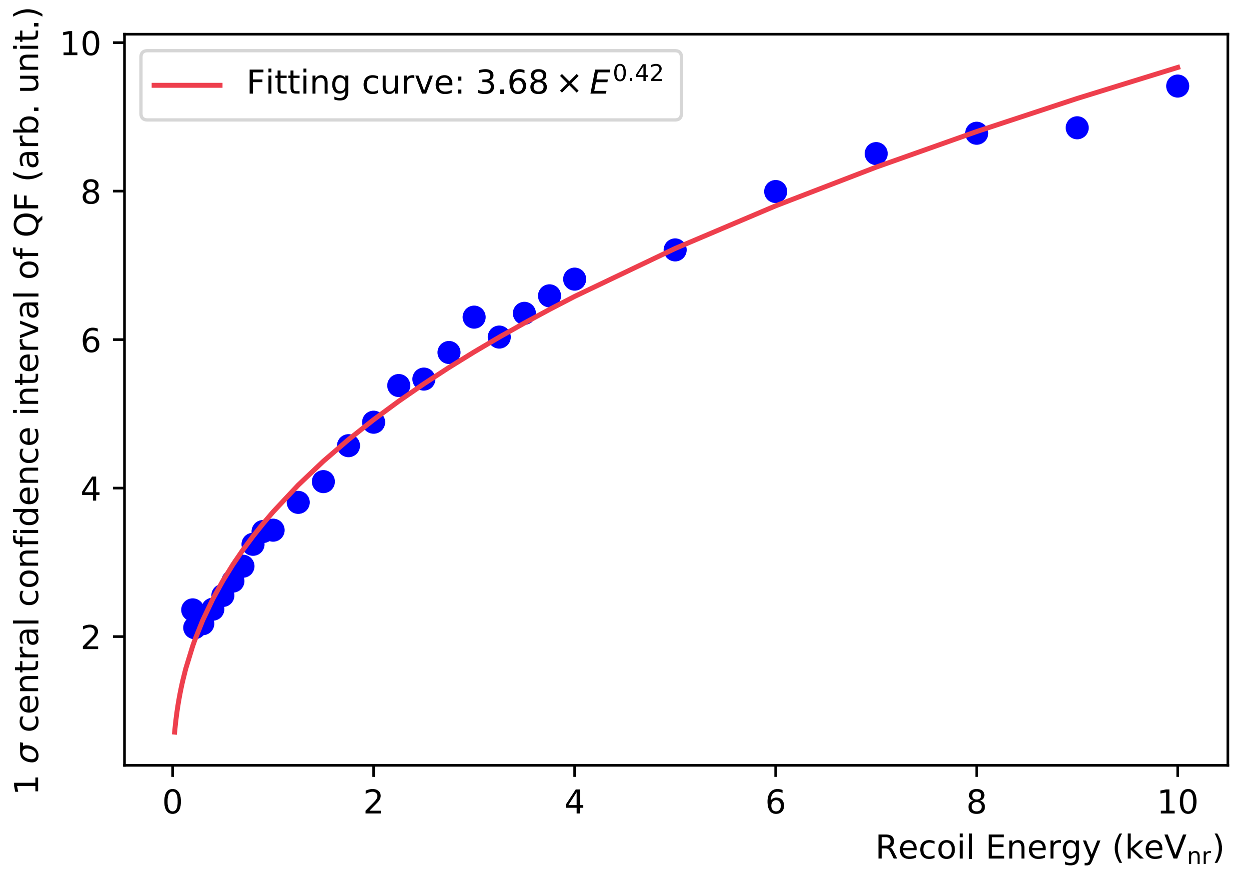
Ionization yield and Its Randomness of Silicon



Calculated mean value of Si QFs compared to measurements and the Lindhard-like models.



Distribution of QFs for keV scale recoil events.

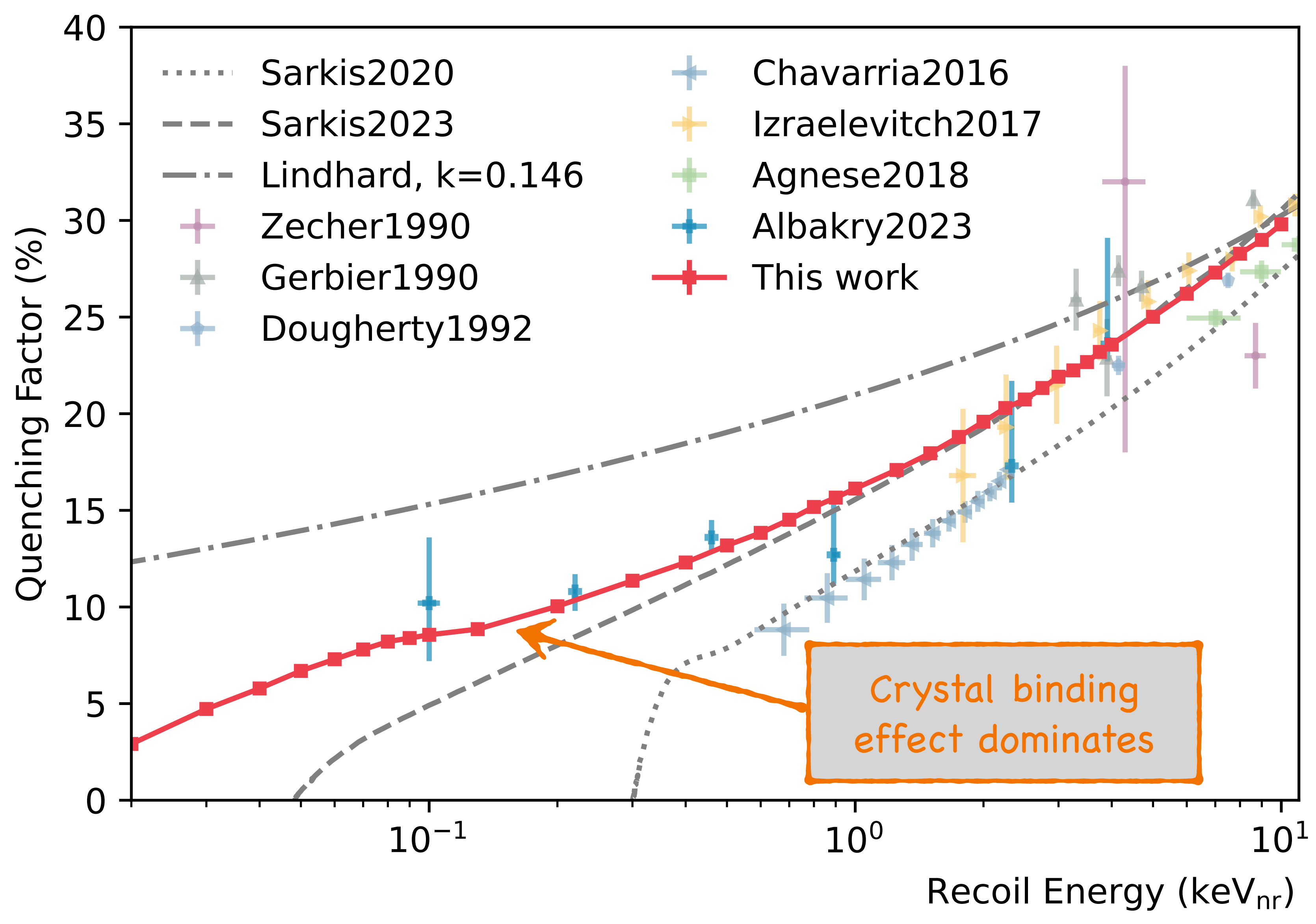


1σ width of ionization distribution as function of recoil energy (> 200 eVnr).

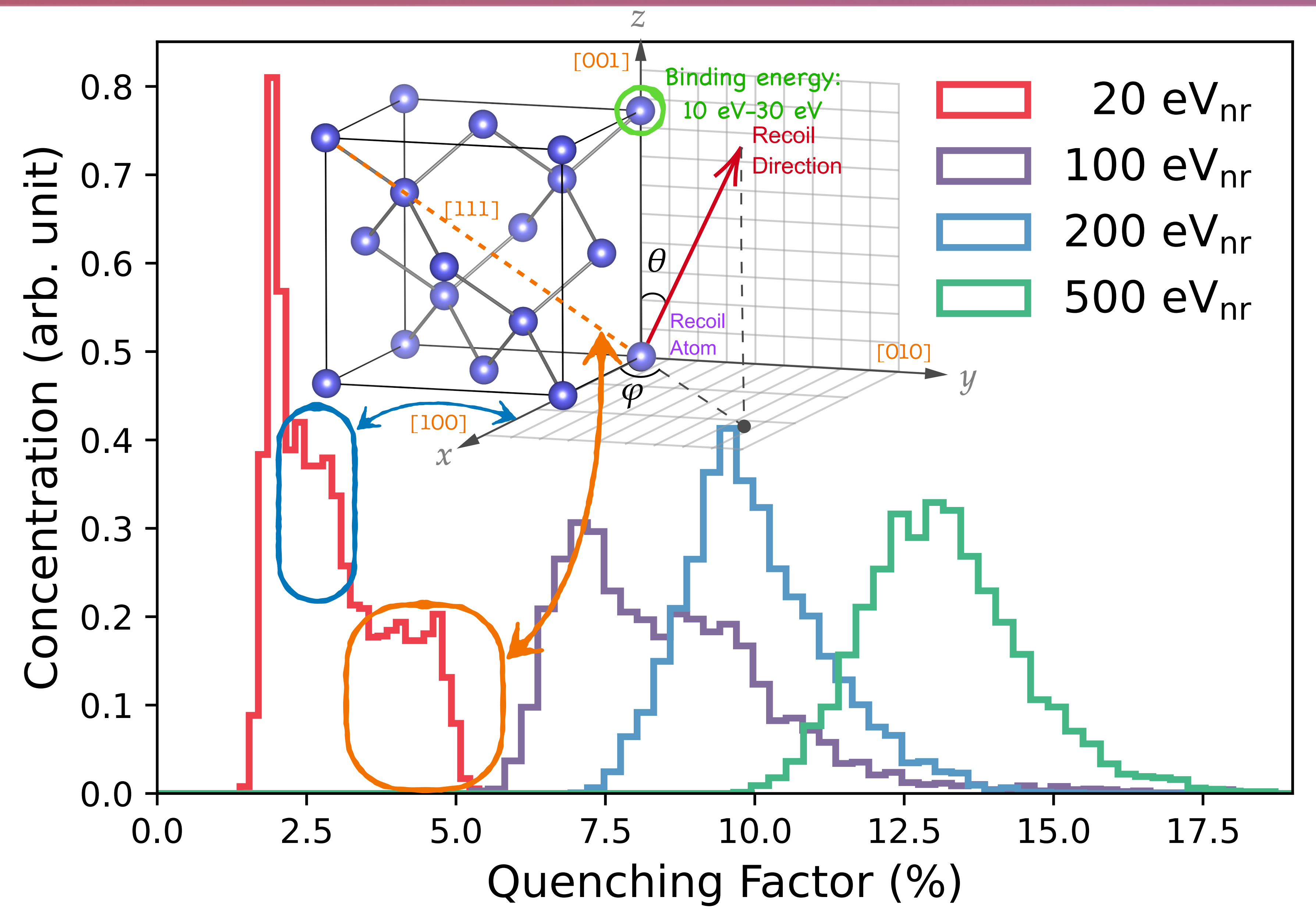
- The results demonstrate a high consistency with the measurements, even at the scale of a single electron-hole pair (EHP).
- Inherent distribution of QFs originates from the random cascade process.
- The broad distribution of QF values indicates that using mean values is insufficient.

Details could be found in: Phys. Rev. D 112, L101303

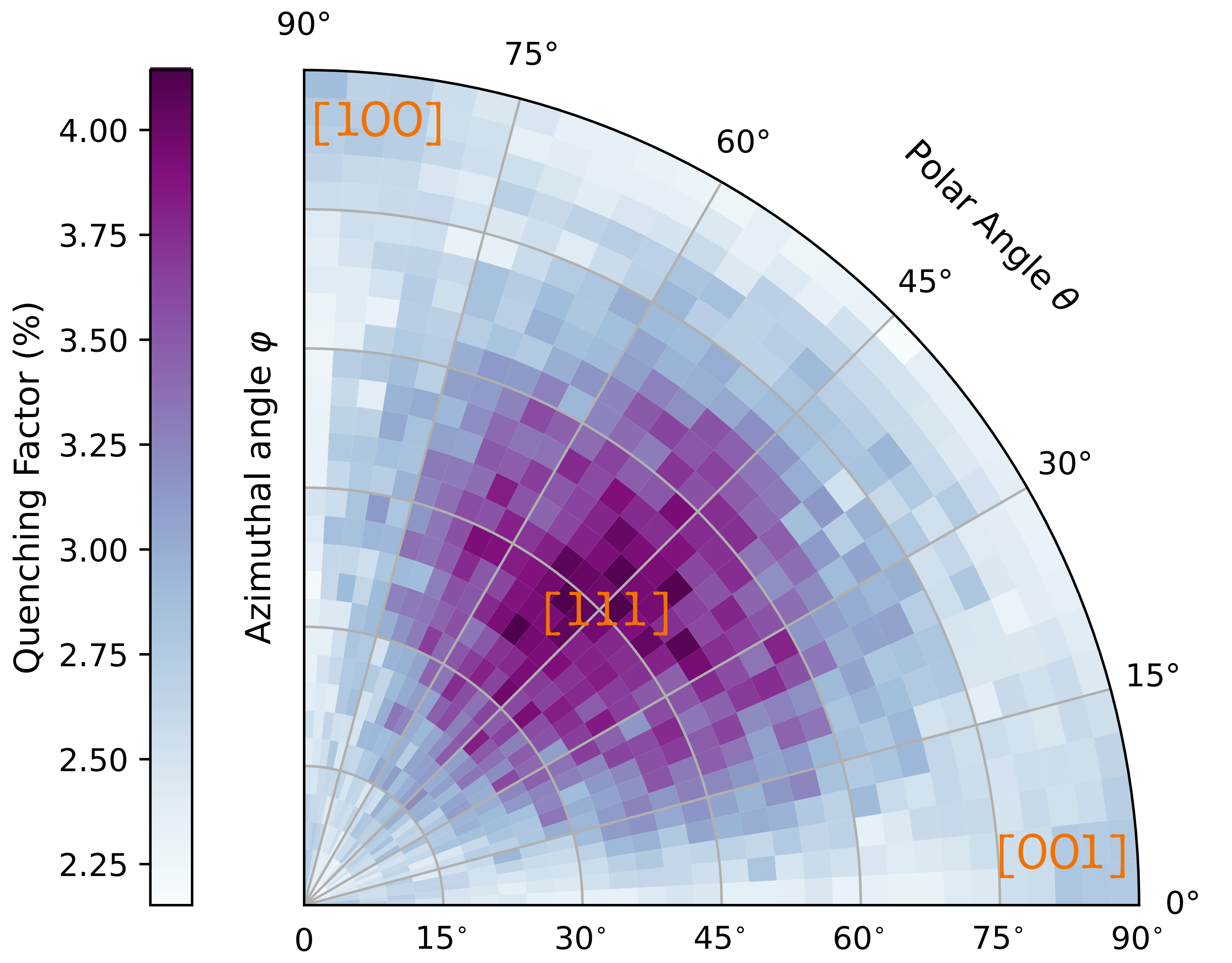
Lattice structure and Low-energy behavior



QF of calculations and measurements.



Distribution of QFs for sub-keV scale recoil events.



Recoil angular dependence of the QF at 20 eVnr, showing mean QF over (θ, φ).

- **Above 10 keVnr** (not shown): Consistence with Lindhard and Sarkis model, indicates binding is not important.
- **From 200 eVnr to 10 keVnr**: Address overestimation of Lindhard model via neglecting binding effect, but no special structure in distribution.
- **Below 200 eVnr**: Lattice binding dominates the QF behavior.

Details could be found in: Phys. Rev. D 112, L101303

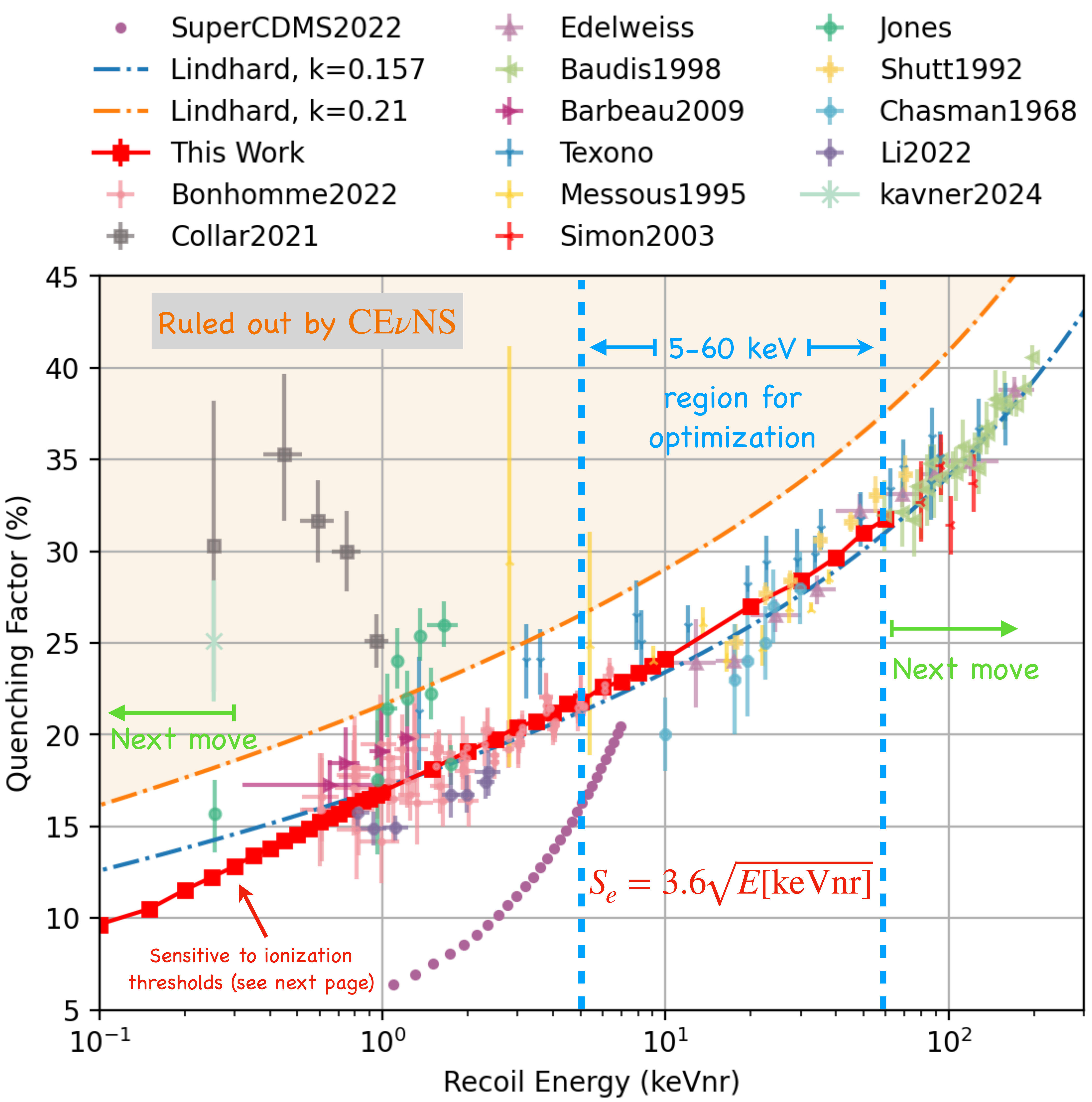
Ionization Yield of Germanium

$$\chi^2 = \frac{(y - f(x))^2}{ey^2 + (\frac{1}{2}(exl + exh)f'(x))^2} \qquad S_e = a\sqrt{E}\ (v < 1\alpha c)$$

	Chi-square	NDF
Texono2009	12.70	9
baudis1998	0.05	1
EDELWEISS	11.07	5
messous1995	44.85	8
shutt1992	17.84	6
bonhomme2022	6.04	8
chasman1968	7.89	6
TOTAL	100.45	43

Chi-square of optimized k for recoil energy from 5 to 60 keVnr.

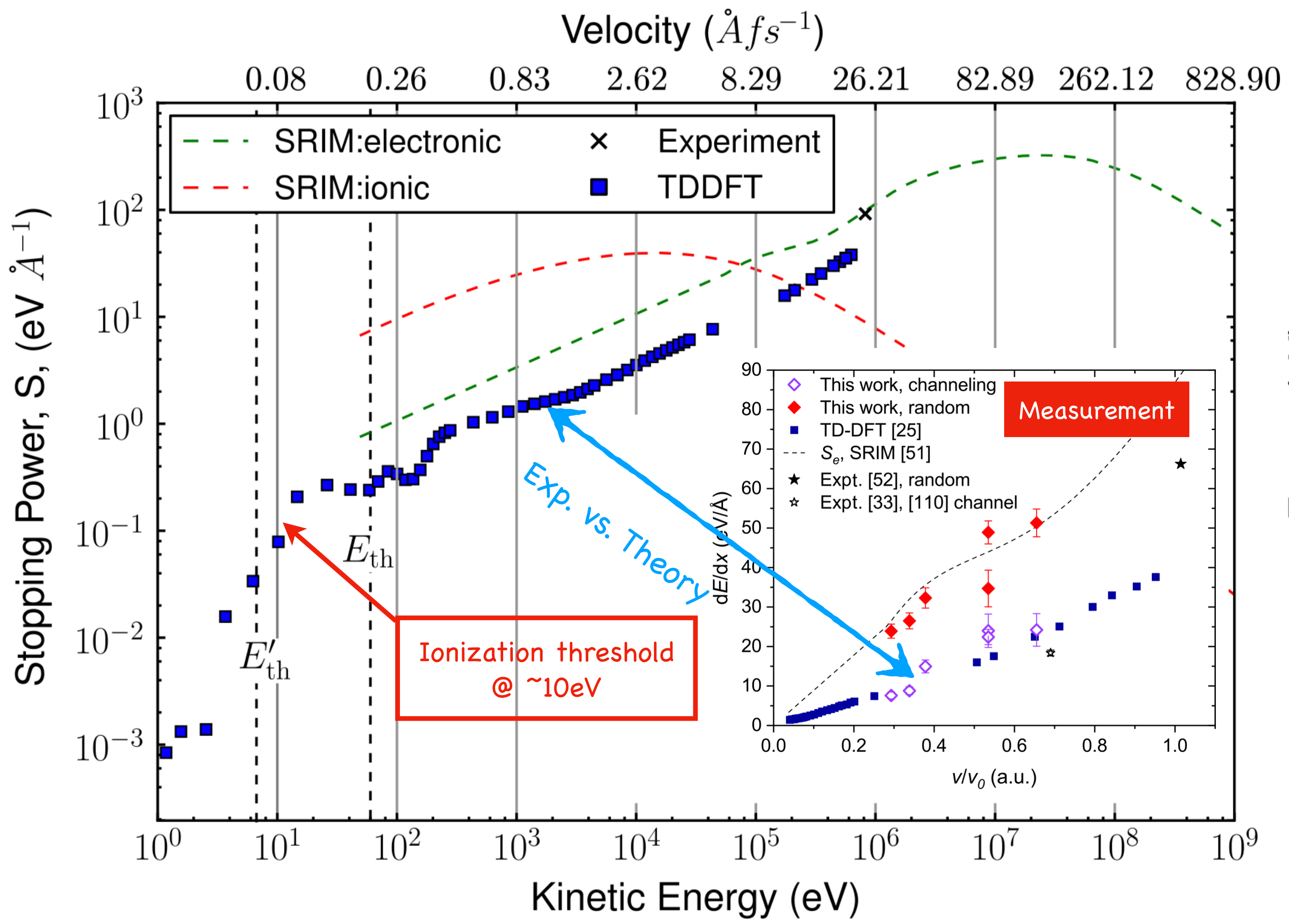
- Binary Search: Optimize the scale factor a of S_e with 7 groups, 43 measurements.
- Extending to high-energy: aligns with the Lindhard model and measurements.
- Consistence with most measurements, but Collar and Kavner's measurements.



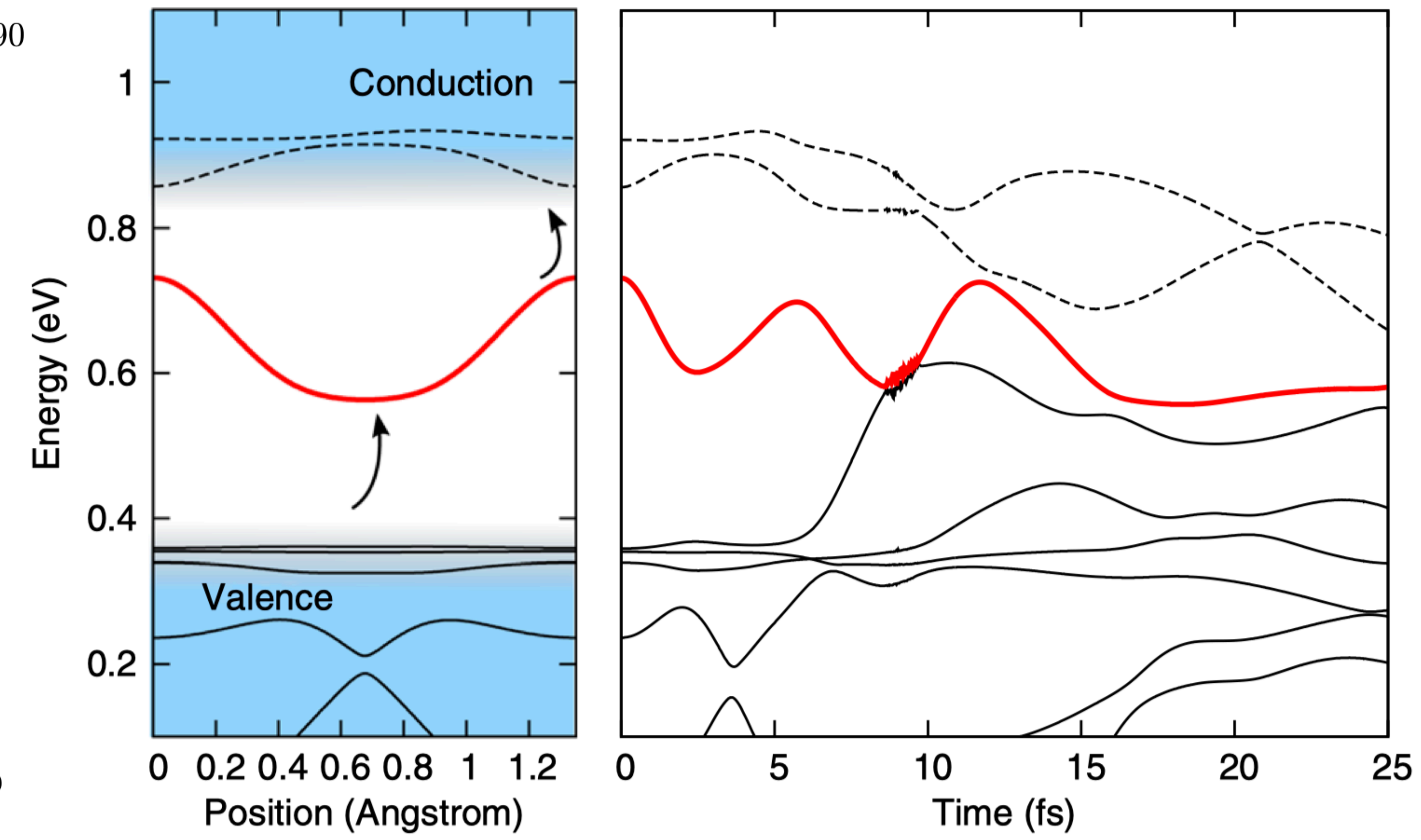
Calculated QF compared to measurements of Ge and the Lindhard models with different parameters. Shadow region is not supported by recent CEvNS results [1-4]

[1] N. Ackermann et al., Direct observation of coherent elastic antineutrino–nucleus scattering, Nature 643, 1229 (2025)
[2] N. Ackermann et al., Final CONUS Results on Coherent Elastic Neutrino-Nucleus Scattering at the Brokdorf Reactor, Phys. Rev. Lett. 133, 251802 (2024)
[3] I. Alekseev et al., First results of the νGeN experiment on coherent elastic neutrino-nucleus scattering, Phys. Rev. D 106, L051101 (2022)
[4] J. Liao, H. Liu, and D. Marfatia, Implications of the first evidence for coherent elastic scattering of reactor neutrinos, Phys. Rev. D 106, L031702 (2022)

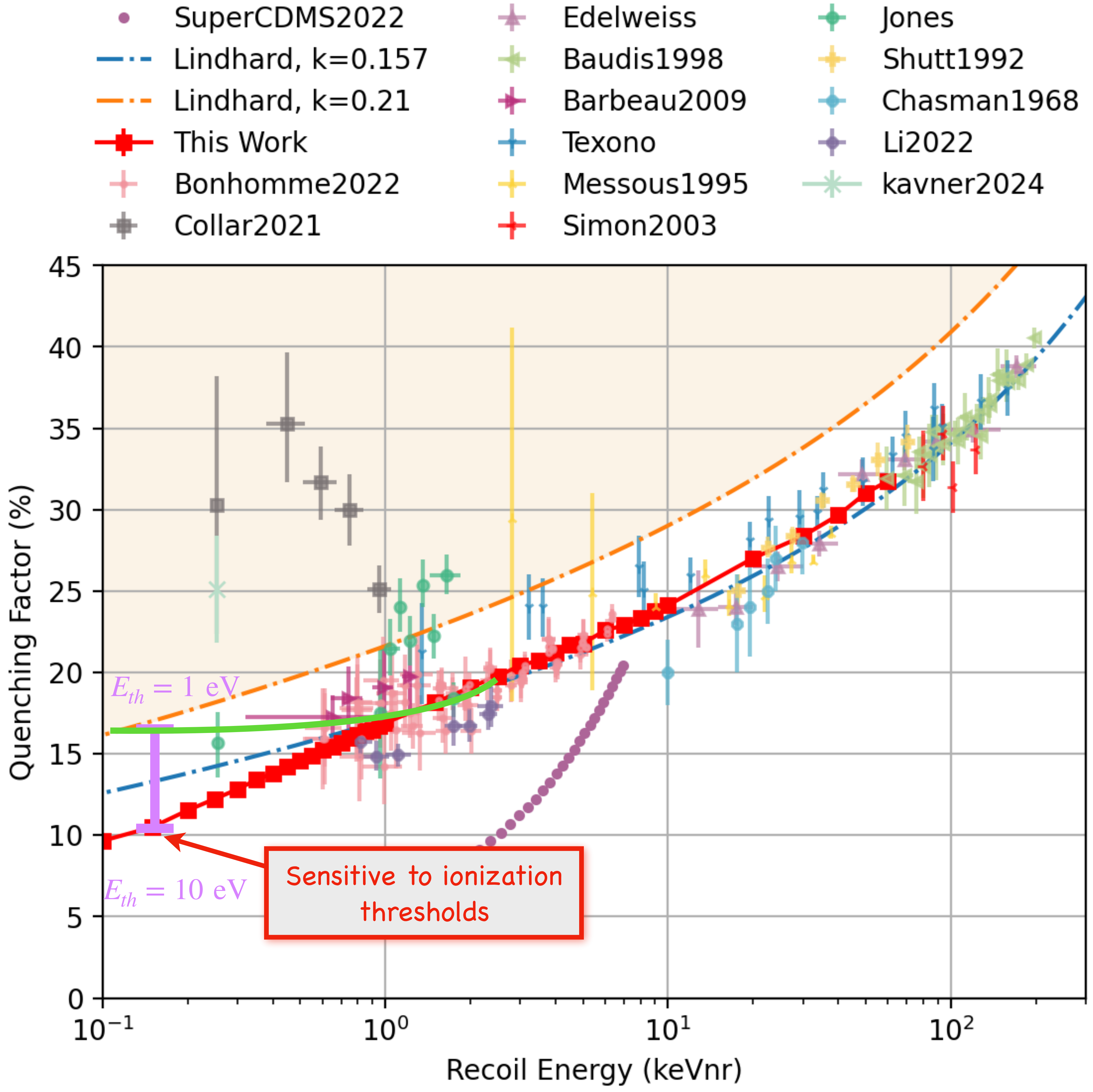
Limitation of Ionization Yield of Nuclear Recoil



Time-dependent density function theory (TDDFT) calculated S_e for Si in Si [1, 2]



The time evolution of mid-gap elevator state (red) as the projectile moves in the crystal [1].

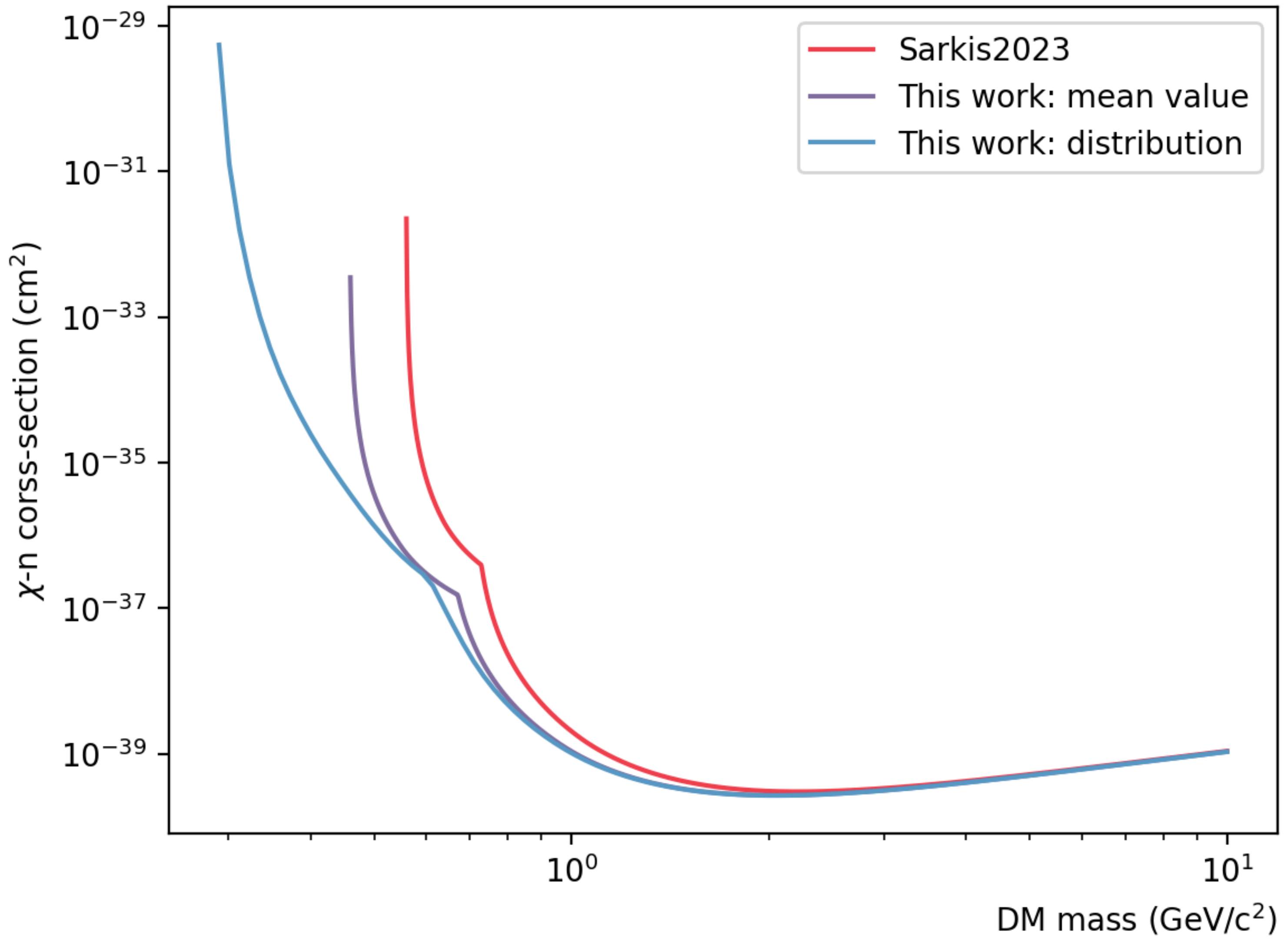


- Ionization threshold (E_{th}) is identified through **ab inito** calculations [1, 2] and experiments [3].
- Incorporating band-gap effects into the nuclear-electron interactions is crucial for QF calculation below ~1 keVnr.
- Cross-check with previously optimized S_e.
- Ab initio calculation for S_e of germanium is on-going.

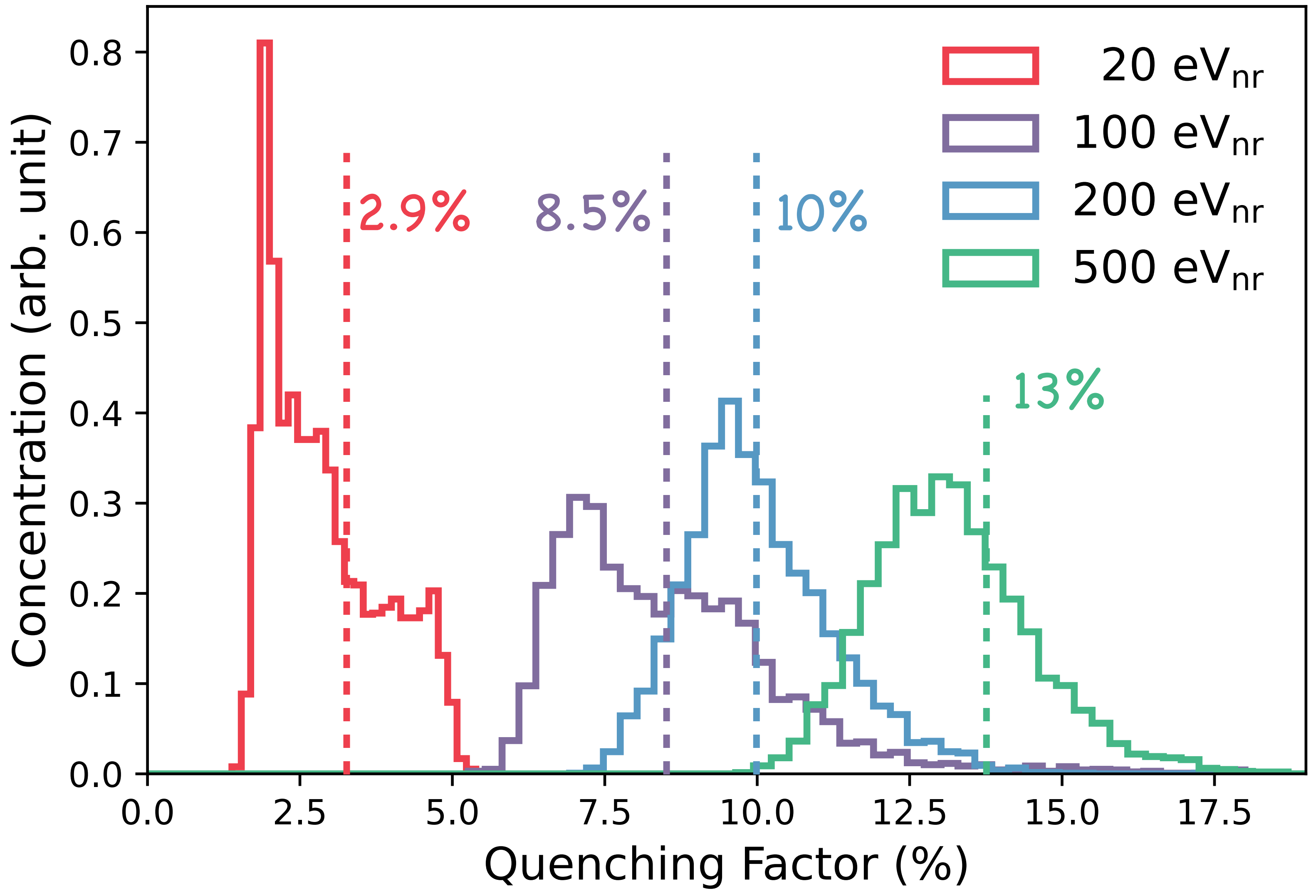
[1] Lim, A. et al. Electron Elevator: Excitations across the Band Gap via a Dynamical Gap State. Phys. Rev. Lett. 116, 043201 (2016).
[2] Lohmann, S., Holeňák, R. & Primetzhofer, D. Trajectory-dependent electronic excitations by light and heavy ions around and below the Bohr velocity. Phys. Rev. A 102, 062803 (2020).
[3] Roth, D. et al. Electronic Stopping of Slow Protons in Oxides: Scaling Properties. Phys. Rev. Lett. 119, 163401 (2017).

- Low-energy Nuclear Recoil and Ionization Quenching
- Molecular Dynamic Approach
- Results and Roadmap for Silicon and Germanium
- **Impact on Dark Matter Searches**
- Summary and Future Prospects

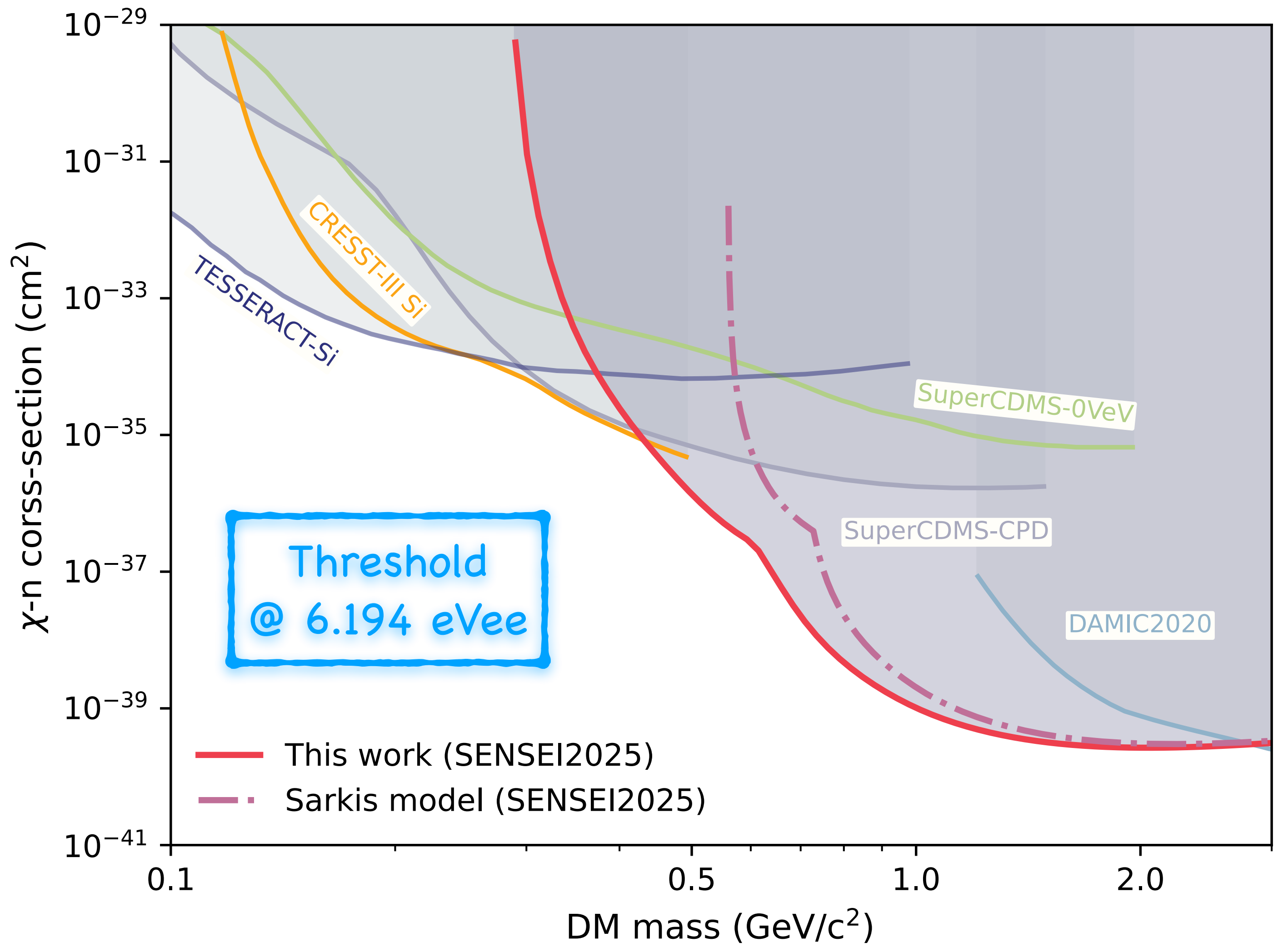
Re-interpretation for sub-GeV Dark Matter Constrain



90% C.L. exclusion limits from SENSEI-2025 via three different QF treatments.



Low-energy events leak to higher Electronic equivalent energy via QF distributions.



90% C.L. upper limits for the χ-N interaction reinterpreted from SENSEI spectrum

- Reinterpreted of SENSEI-2025 (6.194 eVee) [1] with Sarkis model, MD-calculated mean QF, MD-calculated full QF distribution using binned Poisson method.
- Standard DM Halo parameters: $v_{esc} = 544$ km/s, $v_0 = 220$ km/s, $\rho_{DM} = 0.3$ GeV/cm^3/c^2
- Convolution with QF distribution: Enhance sub-GeV constrain, extended exclusion limit to 0.29 GeV/c^2.

[1] P. Adari et al., First Direct-Detection Results on Sub-GeV Dark Matter Using the SENSEI Detector at SNOLAB, Phys. Rev. Lett. 134, 011804 (2025).

Details could be found in: arXiv:2506.03810

- Low-energy Nuclear Recoil and Ionization Quenching
- Molecular Dynamic Approach
- Results and Roadmap for Silicon and Germanium
- Impact on Dark Matter Searches
- **Summary and Future Prospects**

Summary and Prospects

☑ Summary

- Develop a **novel** method to evaluate QFs. Demonstrates good agreement with measurements in silicon even at the level of a single electron-hole pair.
- Considerable width of QF distribution indicating using mean values is **insufficient**. From the distribution perspective constrain on sub-GeV dark mater is extended and enhanced.

☐ Prospects

- Calculation for Germanium still requires more acknowledgement of electronic stopping power, especially for ionization limitation raised by band gaps.
- Confirm the QF distribution with experiments.
- The distribution of the QF might be **universal** in ionization/scintillation detection, as it originates from the random cascade process.

Thank you for your attention!