Learning Loss Functions

BETHANY SUTER, UC BERKELEY

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IN COLLABORATION WITH B. LEHMANN, ARXIV:260X.XXXXX

DM-Electron Absorption & Scattering

- SubGeV DM direct detection is a growing field
- Well-motivated, theoretically & experimentally
- SubGeV DM masses are kinetically matched for electron interactions
- The rate equations for absorption & scattering require the material loss function $\mathcal{W}(q,\omega)$

$$\mathcal{W}(q,\omega) = \mathrm{Im}\left(-\frac{1}{\epsilon(q,\omega)}\right)$$

Dielectric Function

$$\Gamma_{\mathrm{A}} = \kappa^2 m_\chi \mathcal{W}(q \approx 0,\omega)$$

$$\frac{dR}{d\omega} = \frac{\rho_\chi}{2\pi^2 e^2 \rho_T m_\chi} \int dq\, q^3 |V(q)|^2 \mathcal{W}(q,\omega)\eta(v_{min}(q,\omega))$$

1608.01994
2104.12786
2101.08263

Where might we find the next-gen sub-GeV DM detector material(s)?

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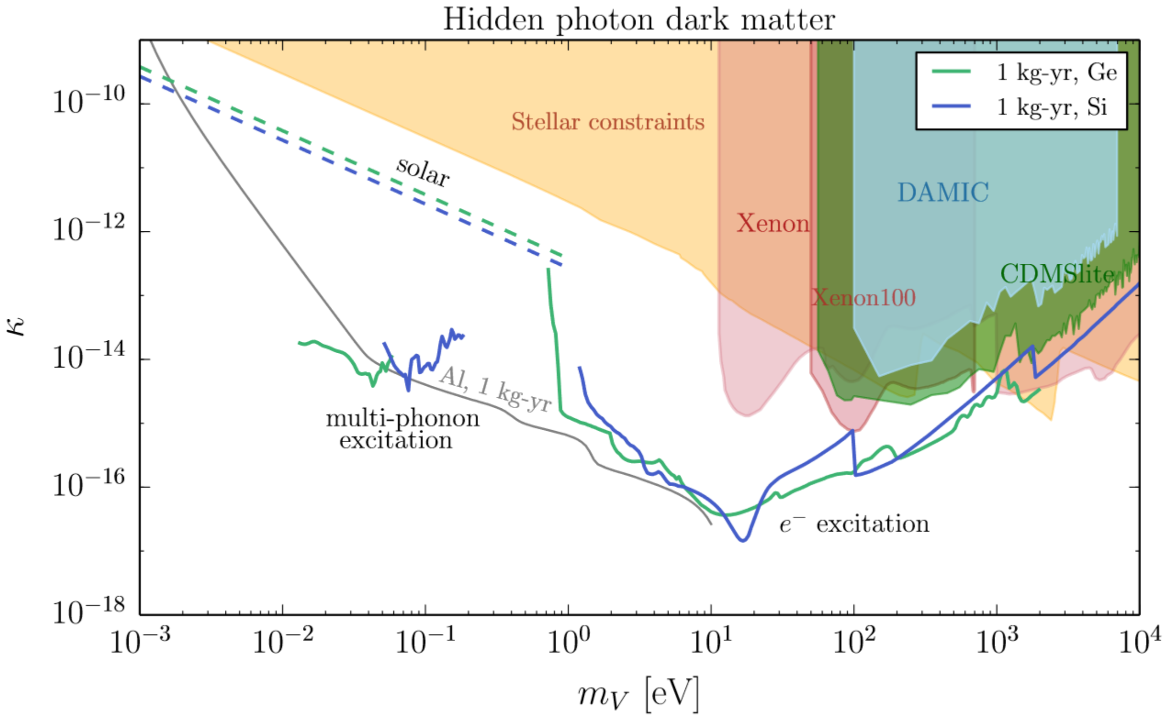
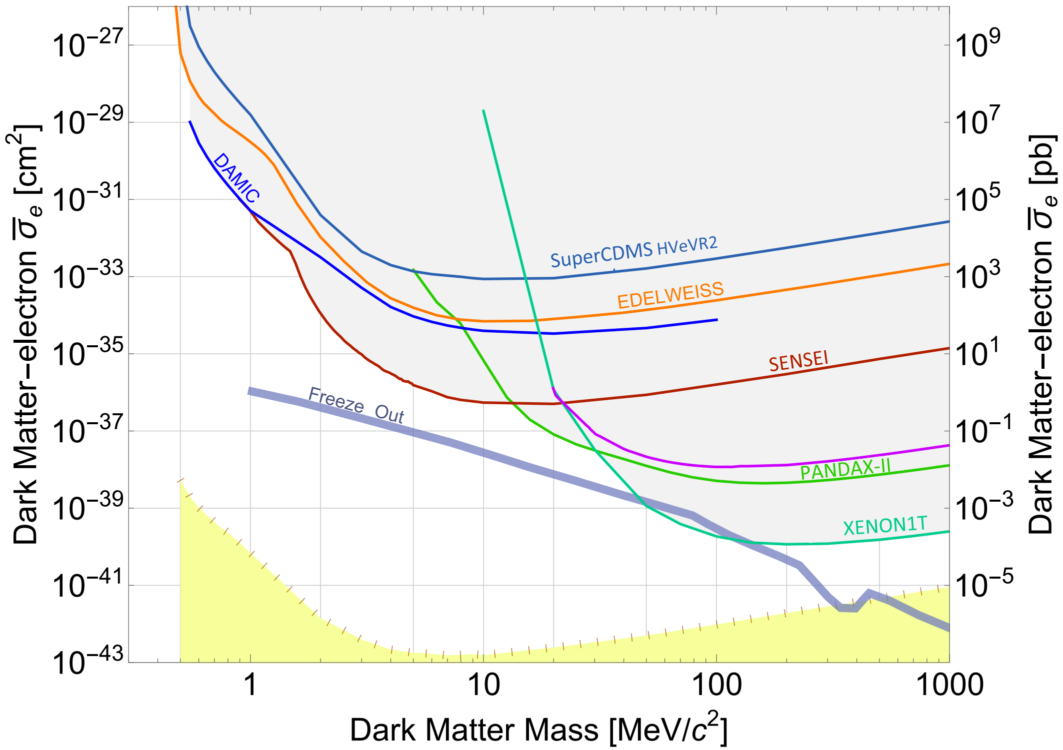
10s of well-known materials with experimentally measured properties

Current DM-Electron Detector Reaches

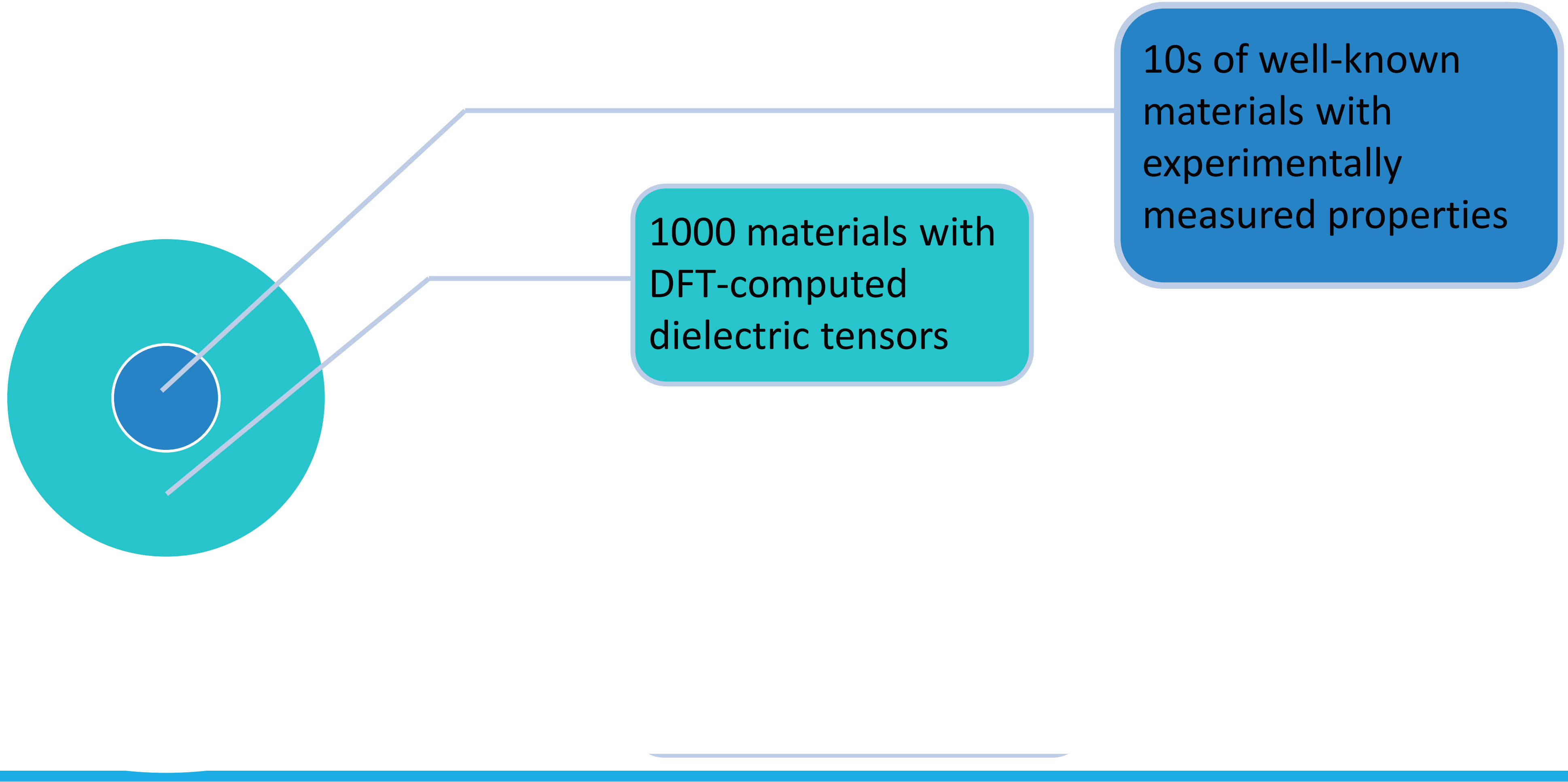


arXiv:1608.01994



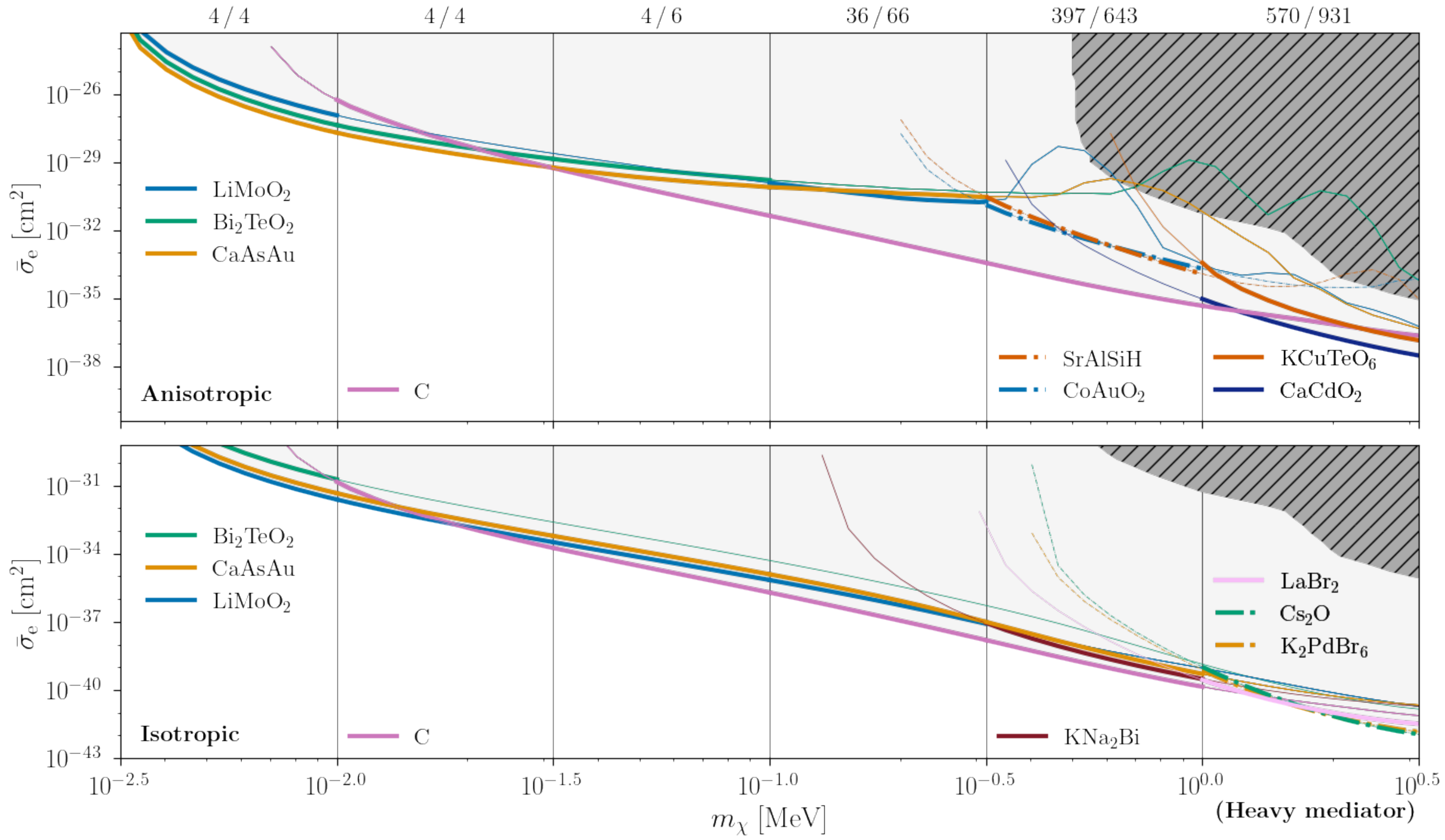
Credit: SuperCDMS DM Limit Plotter

Where might we find the next-gen sub-GeV DM detector material(s)?



10s of well-known materials with experimentally measured properties

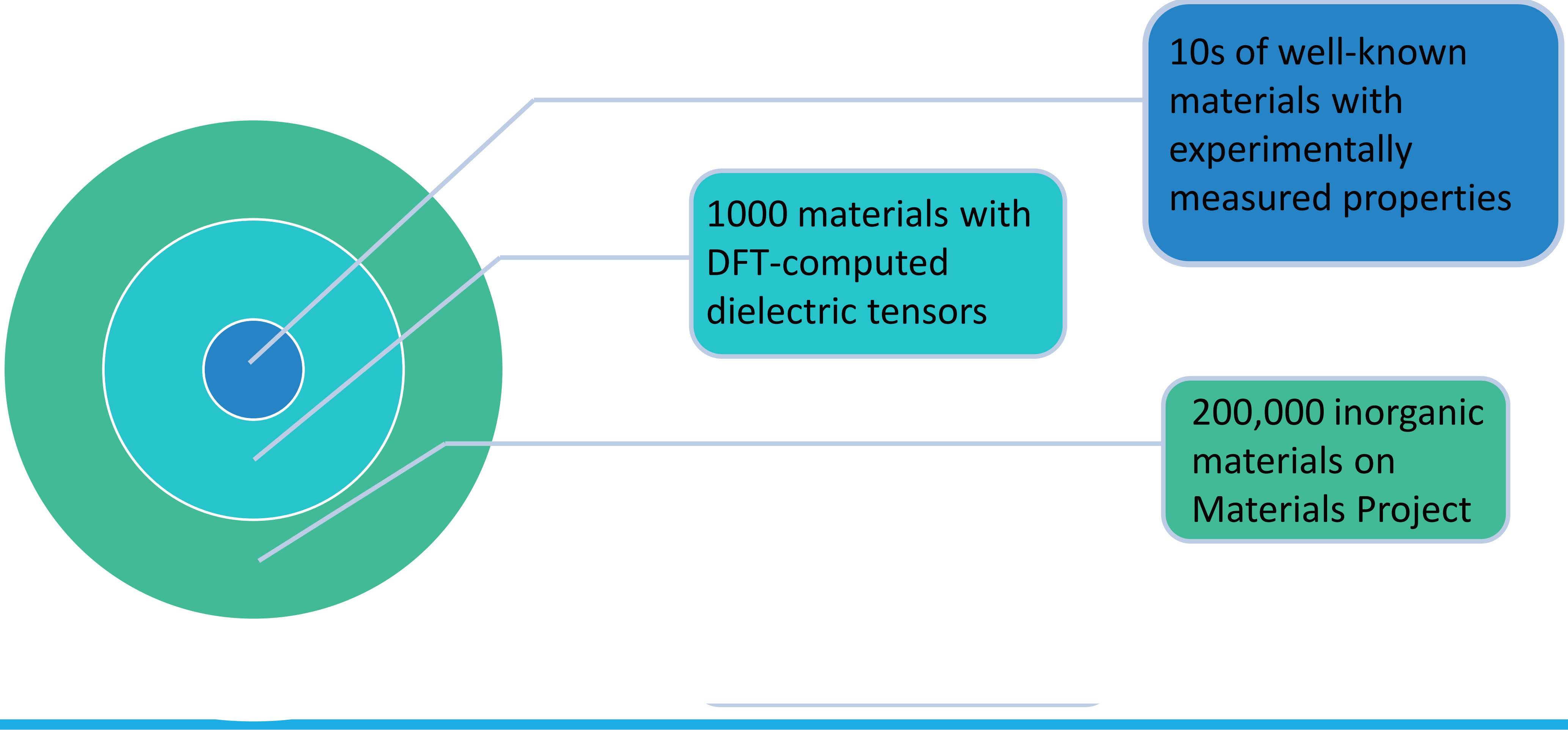
1000 materials with DFT-computed dielectric tensors



- In 2506.19905, I analyzed 986 materials with DFT-computed dielectric tensors
- 593 materials with significant anisotropy
- Computed absorption, DM-electron scattering, and daily modulation curves

Previously On… Pheno 2025

Where might we find the next-gen sub-GeV DM detector material(s)?

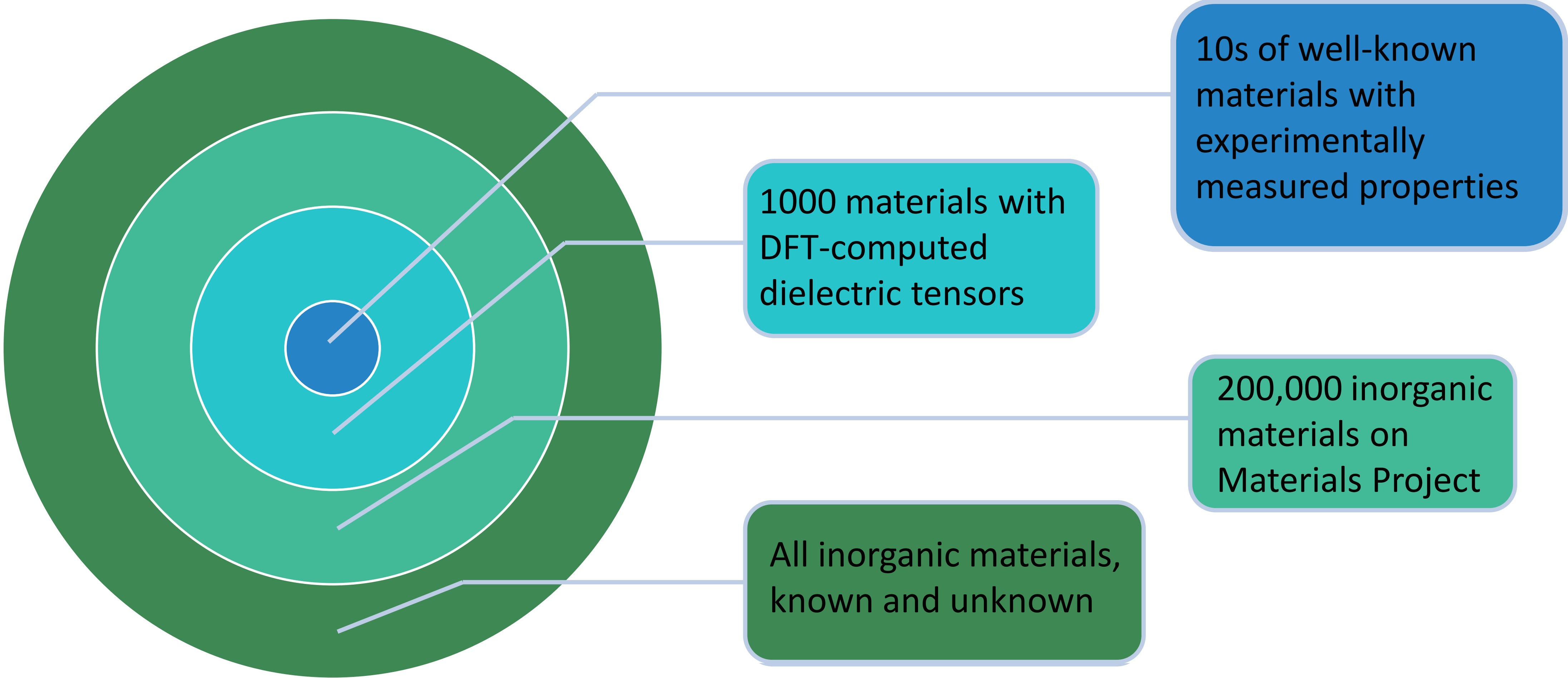


10s of well-known materials with experimentally measured properties

1000 materials with DFT-computed dielectric tensors

200,000 inorganic materials on Materials Project

Where might we find the next-gen sub-GeV DM detector material(s)?



10s of well-known materials with experimentally measured properties

1000 materials with DFT-computed dielectric tensors

200,000 inorganic materials on Materials Project

All inorganic materials, known and unknown

Graph Neural Network for Optical spectra prediction (GNNOpt)

- Only requires the crystal structure as input
- Incorporates three atomic features (atomic mass, dipole polarizability, & covalent radius
- Outputs optical spectra like the dielectric function
- Limitations:
  - Limited to eV scale energy deposits
  - Doesn’t predict anisotropy in materials

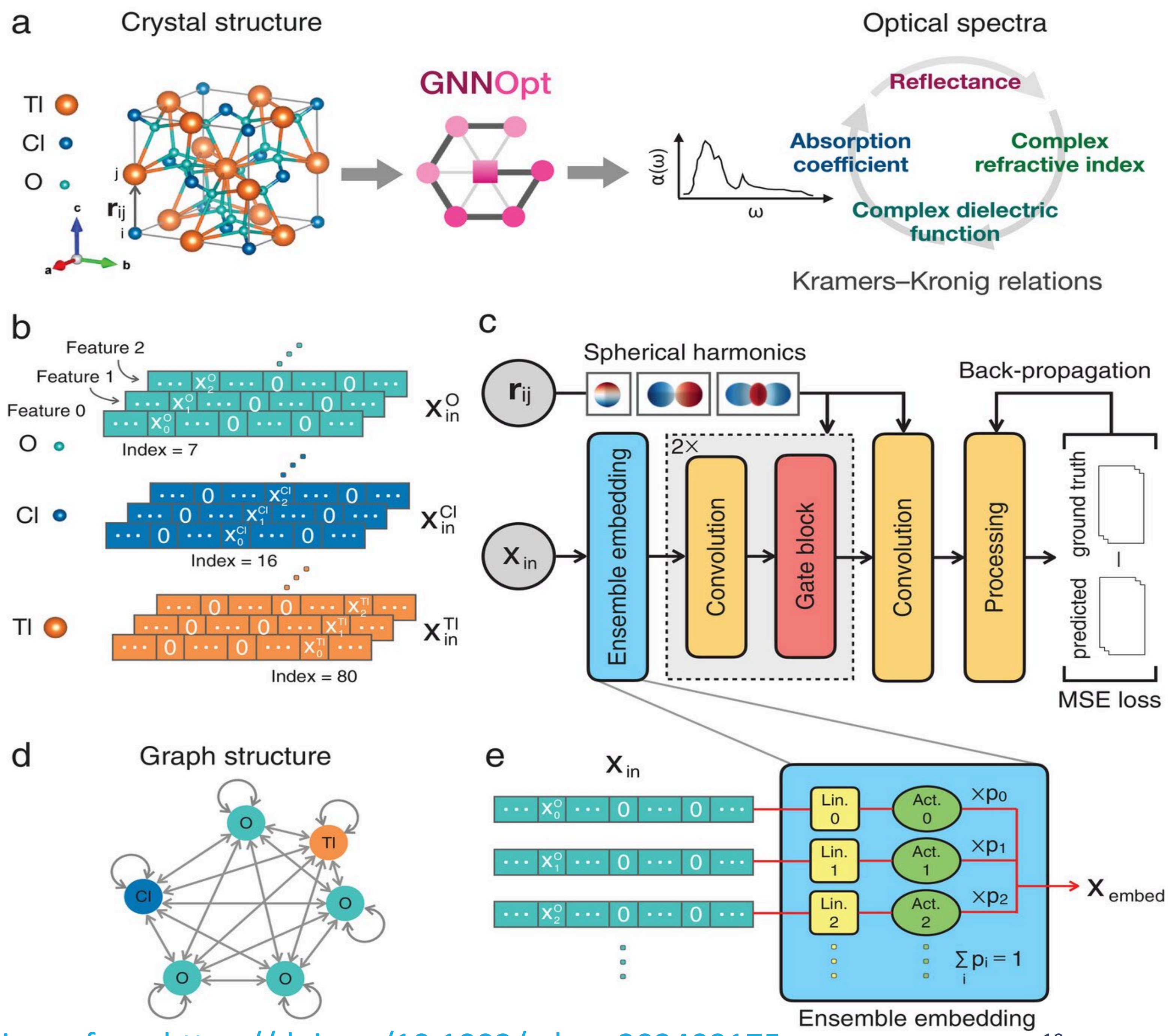


Figure from https://doi.org/10.1002/adma.202409175

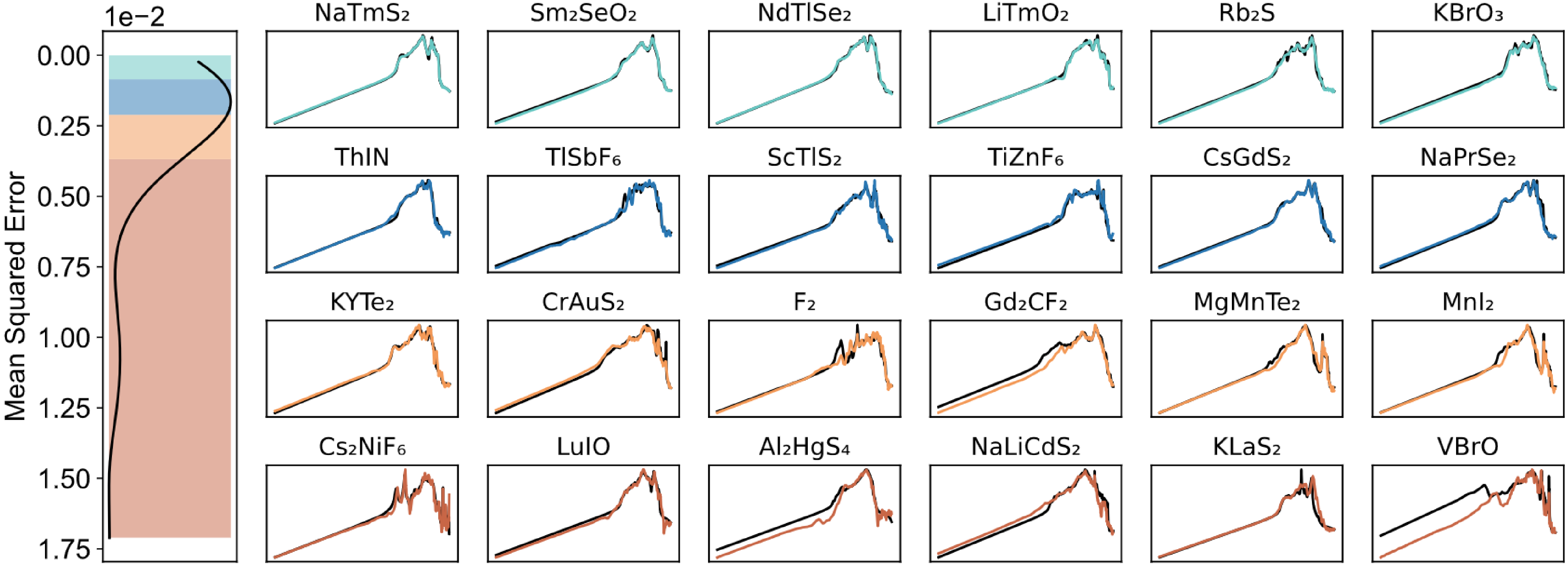
Our Modifications to GNNOpt

- Trained on smaller energy deposits ($\omega \sim 1\ meV$)
- Log-scaled the outputs

$$\mathrm{Im}[\epsilon(\omega)] \rightarrow \mathrm{Log}_{10}(\mathrm{Im}[\epsilon(\omega)])$$
$$\mathrm{Re}[\epsilon(\omega)] \rightarrow \mathrm{Symlog}_{10}(\mathrm{Re}[\epsilon(\omega)])$$

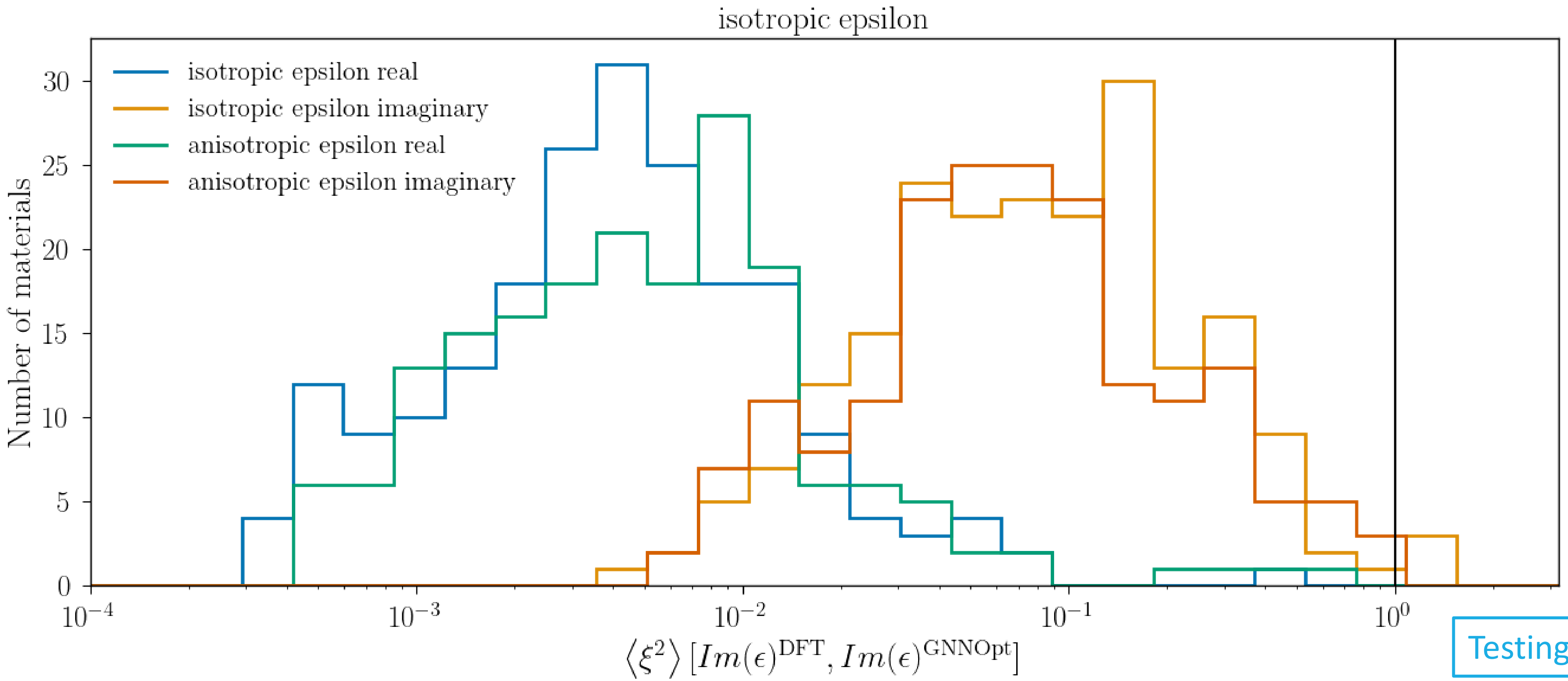
- Changed the model to allow training of anisotropic materials
- Trained to different steps in the process
  - dielectric function, dielectric tensor, loss function, isotropic reach curves, anisotropic reach curves
- Incorporated the outputs into our pipeline to determine the projected reach curve for each material

Performance of GNNOpt on Loss Test Dataset



Isotropic Epsilon

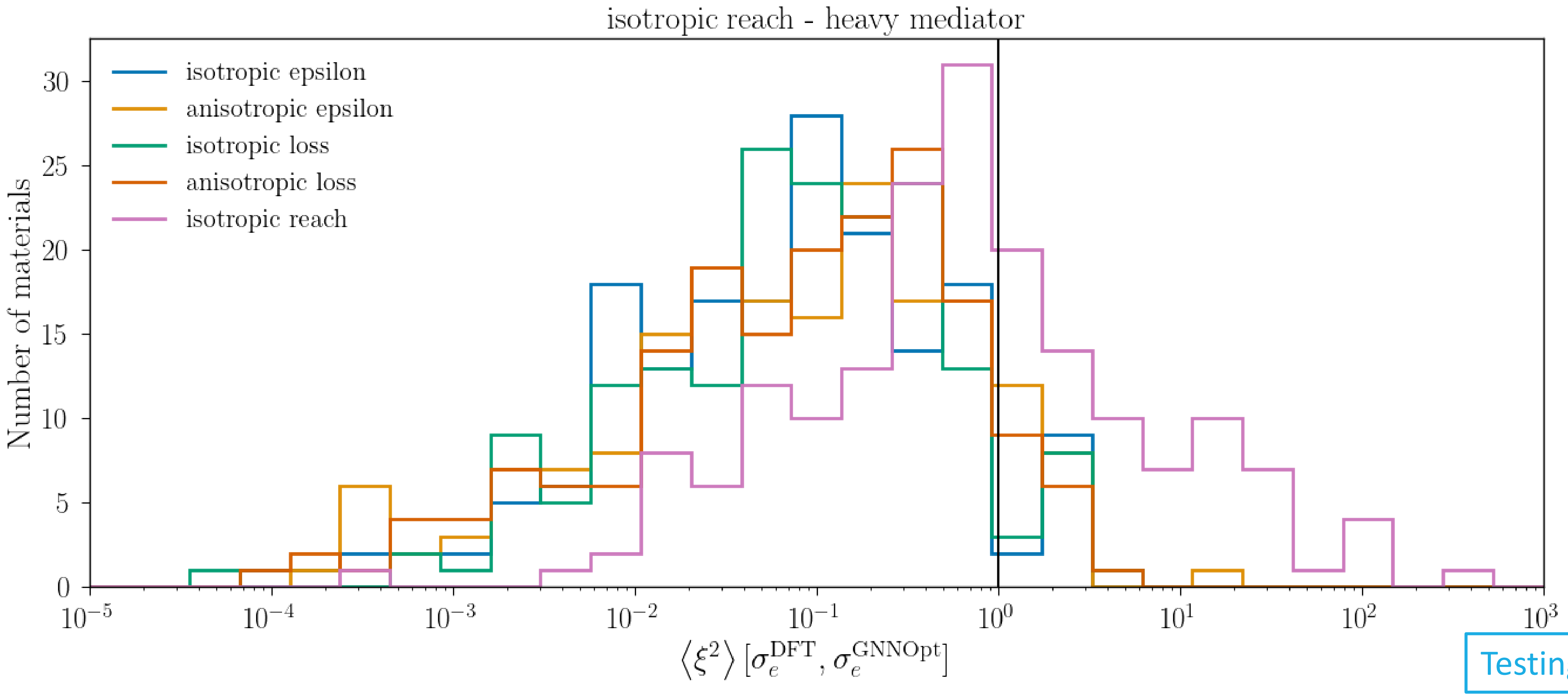
$$\langle\xi^2\rangle[X^{DFT}, X^{GNNOpt}] = \sum_i^N \frac{\left[\log_{10}(X_i^{DFT}) - \log_{10}(X_i^{GNNOpt})\right]^2}{N}$$



Testing set only

Isotropic Reach

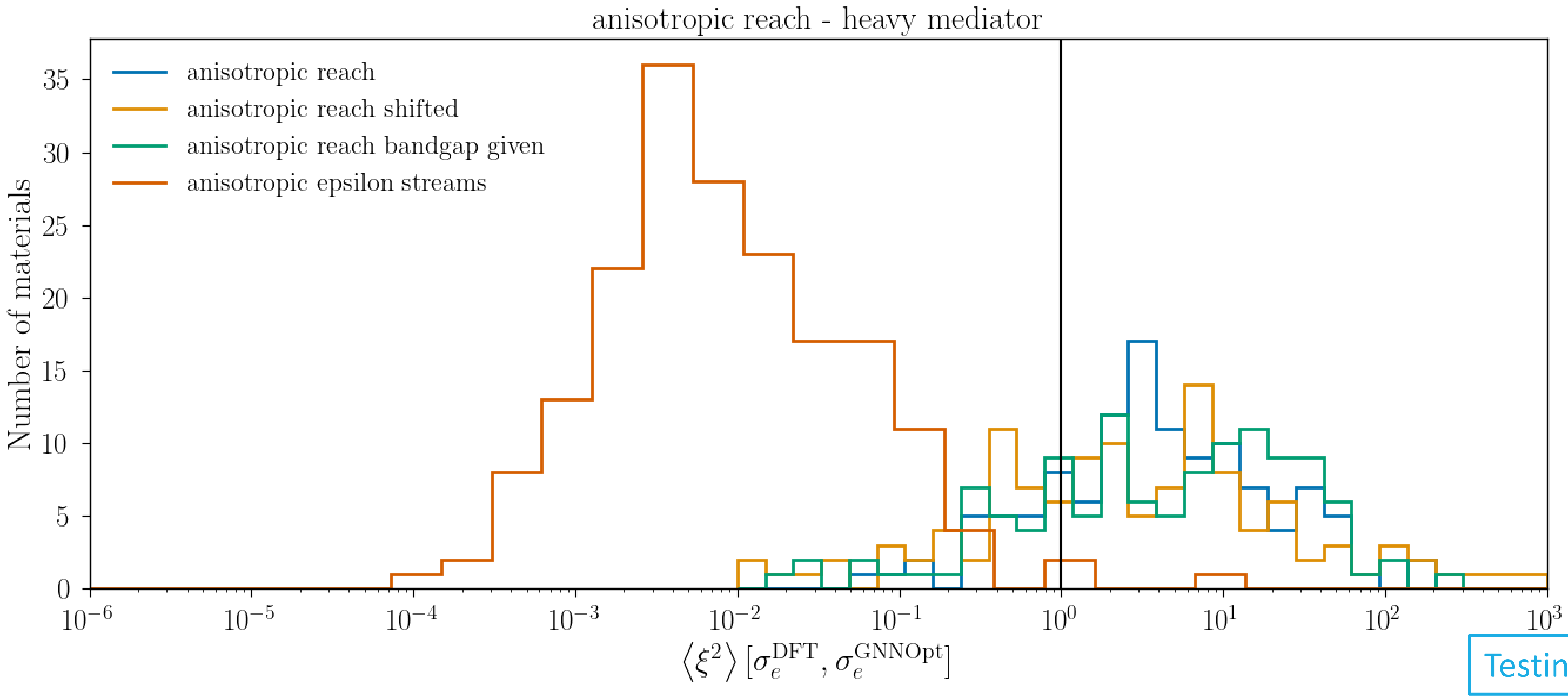
$$\langle\xi^2\rangle[X^{DFT}, X^{GNNOpt}] = \sum_i^N \frac{\left[\log_{10}\left(X_i^{DFT}\right) - \log_{10}\left(X_i^{GNNOpt}\right)\right]^2}{N}$$



Testing set only

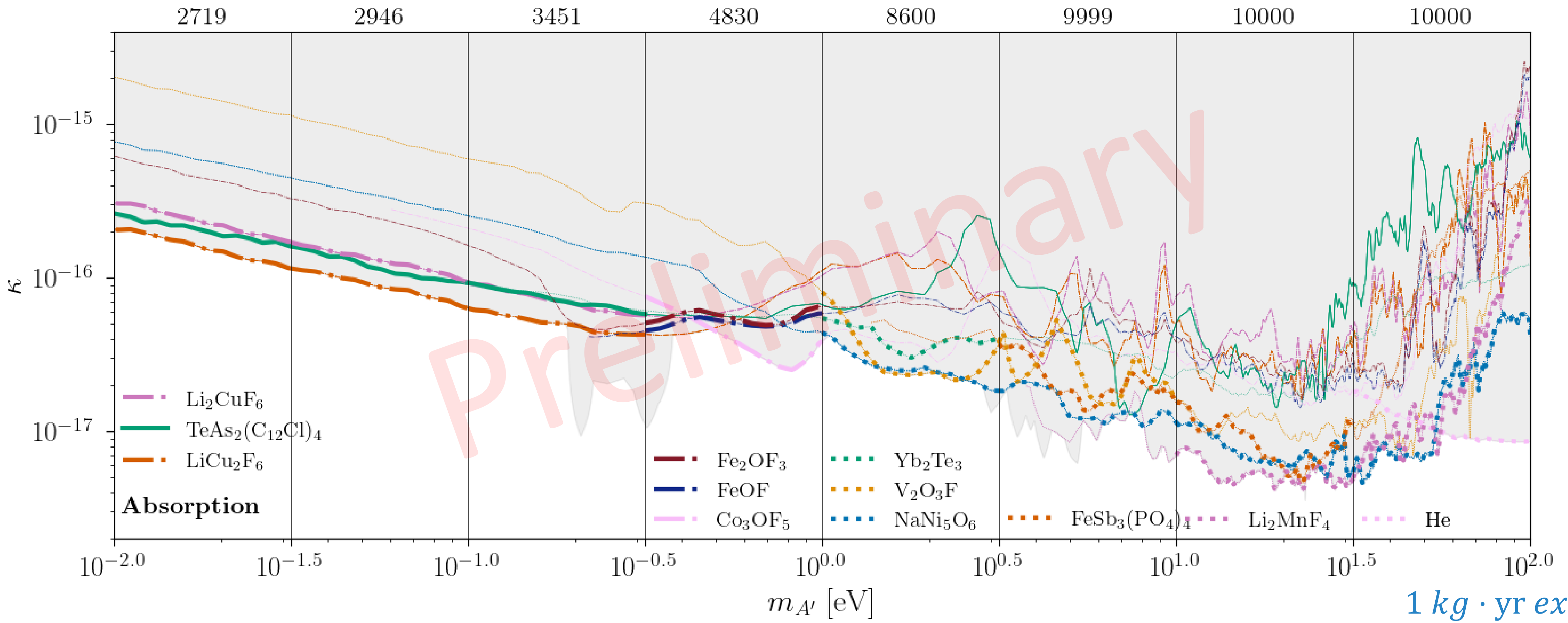
Anisotropic Reach

$$\langle \xi^2 \rangle [X^{DFT}, X^{GNNOpt}] = \sum_{i}^{N} \frac{\left[\log_{10}(X_i^{DFT}) - \log_{10}(X_i^{GNNOpt})\right]^2}{N}$$



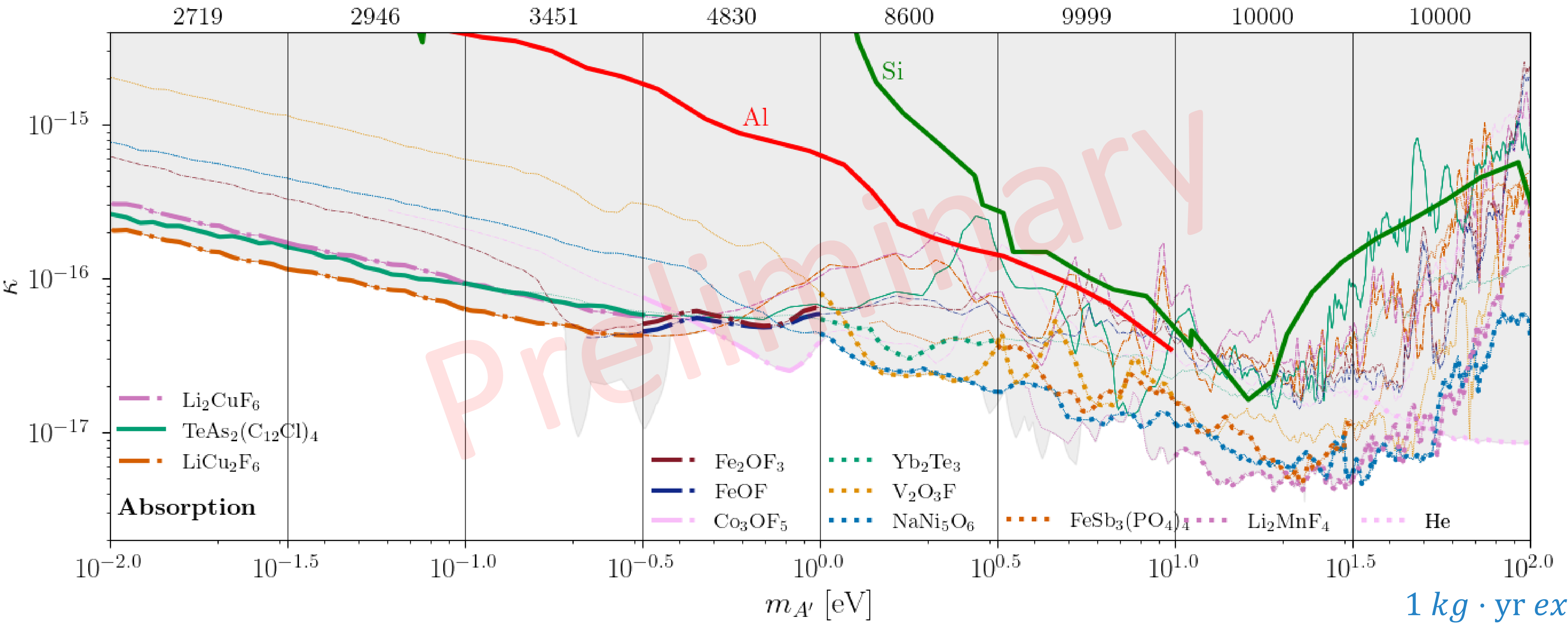
Testing set only

Absorption



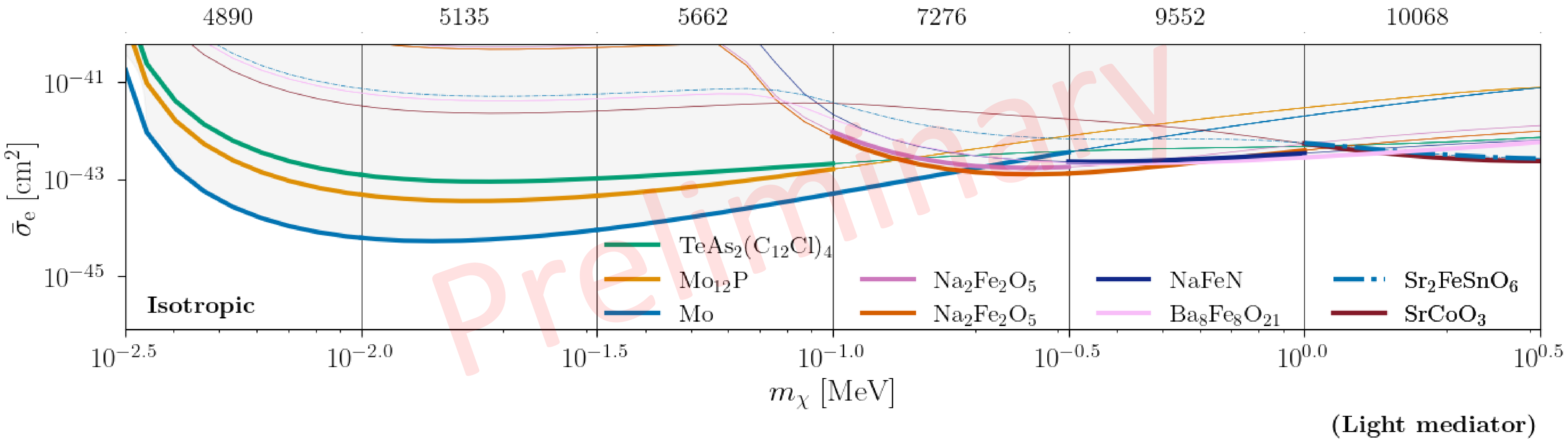
$1\ kg \cdot yr\ exposure$

Dark Photon Absorption



$1\ kg \cdot yr\ exposure$

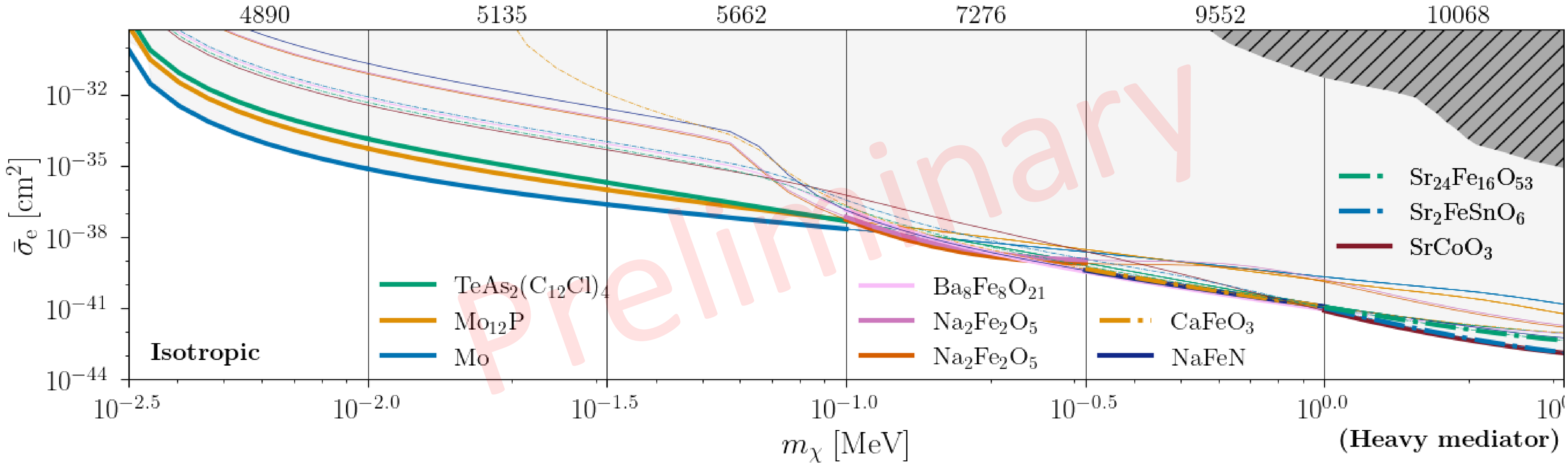
DM-Electron Scattering - Light Mediator



$1\ kg \cdot yr\ exposure$

$E_{th} = 10\ meV$

DM-Electron Scattering - Heavy Mediator



$1\ kg \cdot yr\ exposure$

$E_{th} = 10\ meV$

Conclusions

We analyze 10,000 (and in the future, over 100,000) inorganic materials to determine optimal candidates for future subGeV DM experiments

We use the GNNOpt ML architecture with basic modifications to predict dielectric tensors, loss functions and reach curves for all 10,000(0) materials.

Since the only required input is the material structure, this model can quickly produce results for any inorganic material of interest.

The ML model predictions are robust at the percent level, even when modeling anisotropic dielectric tensors/losses.

Questions?

Backup Slides

DM-Electron Absorption Rate

Kinetic mixing coupling between dark photon and SM photon

Dark matter mass

$$\Gamma_{\mathrm{A}} = \kappa^2 m_\chi \mathcal{W}(q \approx 0, \omega)$$

Loss function of the material

$$\mathcal{W}(q, \omega) = \operatorname{Im}\left(-\frac{1}{\epsilon(q \approx 0, \omega)}\right)$$

Dielectric Function:
Parametrizes a material's response to deposits of energy/momentum

DM-Electron Scattering Rate

Non-relativistic DM-electron potential

$$V(q) = \frac{g_\chi g_e}{q^2 + m_{\phi,V}^2}$$

Mean inverse DM speed (via SHM)

$$\eta(v_{min}) = \int_{v_{min}} d^3\boldsymbol{v}_\chi \frac{f(\boldsymbol{v}_\chi)}{v_\chi}$$

$$\frac{dR}{d\omega} = \frac{\rho_\chi}{2\pi^2 e^2 \rho_T m_\chi}\int dq\, q^3 |V(q)|^2 \mathcal{W}(q,\omega)\,\eta(v_{min}(q,\omega))$$

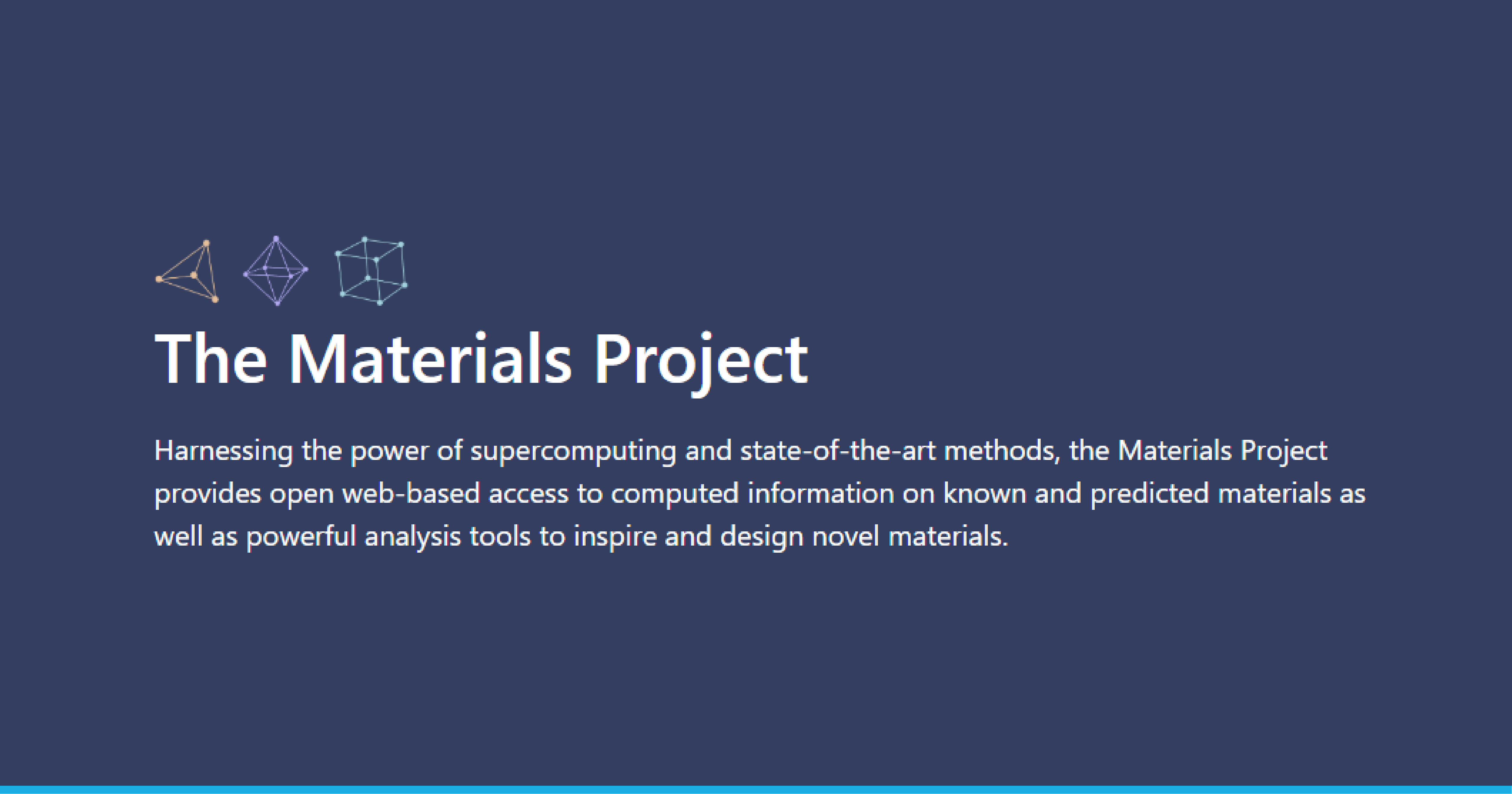
Mass density of the target material

Loss function of the material

$$\mathcal{W}(q,\omega) = \operatorname{Im}\left(-\frac{1}{\hat{q}.\overleftrightarrow{\epsilon}(q,\omega).\hat{q}}\right)$$

Kinematic constraint

$$v_{min} = \frac{\omega}{q} + \frac{q}{2m_\chi}$$

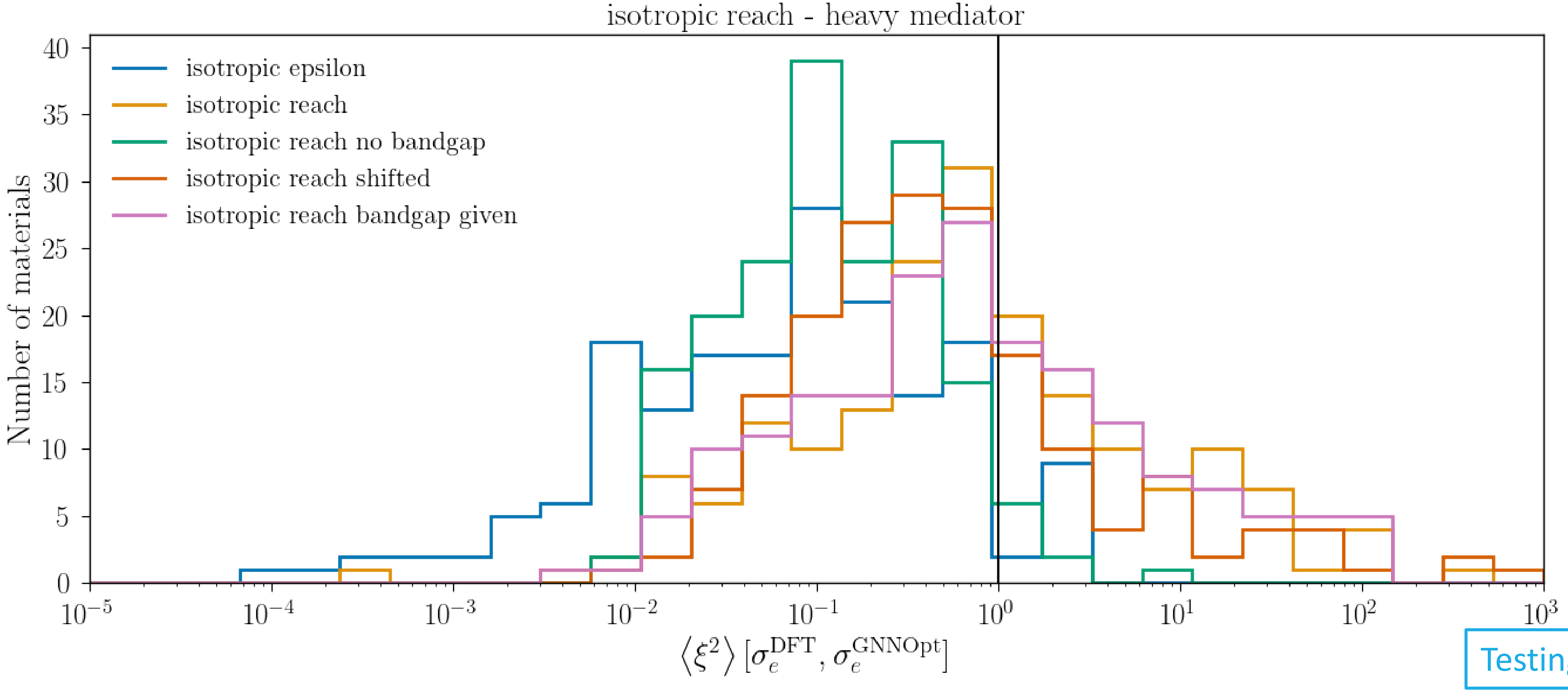


The Materials Project

Harnessing the power of supercomputing and state-of-the-art methods, the Materials Project provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.

Isotropic Reach

$$\langle \xi^2 \rangle [X^{DFT}, X^{GNNOpt}] = \sum_i^N \frac{\left[\log_{10}(X_i^{DFT}) - \log_{10}(X_i^{GNNOpt})\right]^2}{N}$$



Testing set only

How to Extract Momentum Dependence

- The Lindhard Dielectric Function has momentum dependence:

$$\epsilon_{RPA}(q,\omega) = 1 + \frac{3\omega_p^2}{q^2 v_F^2}\left\{\frac{1}{2} + \frac{k_F}{4q}(1 - Q_-^2)\mathrm{Log}\left(\frac{Q_- + 1}{Q_- - 1}\right) + \frac{k_F}{4q}(1 - Q_+^2)\mathrm{Log}\left(\frac{Q_+ + 1}{Q_+ - 1}\right)\right\}$$

  - Derived using perturbation theory and the Random Phase Approximation (RPA)
  - Models materials with one plasmon peak very well

$$Q_\pm = \frac{q}{2k_f} \pm \frac{\omega + i\,\Gamma_p}{q v_f}$$

- We can fit the $q \to 0$ limit to the Materials Project dielectric functions and extract ω_p and Γ_p:

$$\epsilon_{RPA}(q \to 0, \omega) = 1 + \frac{\omega_p^2}{\left(\Gamma_p - i\omega\right)^2}$$

k_f, v_f can be derived from ω_p

Full Pipeline

1. Locations of peaks, ω_p, are determined by zeros in Re(ϵ)
2. We fit a sum of loss functions at q=0:

$$W_{fit}(q,\omega) = \frac{1}{\sum_k h_k} \sum_{k=}^{n_{peaks}} h_k\, Im\left(-\frac{1}{\epsilon_L\left(\omega_{p,k},\Gamma_{p,k};q,\omega\right)}\right)$$

3. We define $r(\omega) = \frac{W_{data}(\omega)}{W_{fit}(q=0,\omega)}$ and assume all features not described by Lindhard plasmons are independent of q
4. We calculate the scattering rate using

$$W(q,\omega) = r(\omega)\, W_{fit}(q,\omega)$$

For anisotropic materials, repeat this process for $\hat{q}.\overleftrightarrow{\epsilon}(q,\omega).\hat{q}$ with $\hat{q}$ pointing uniformly around the unit sphere

Full Pipeline

1. Locations of peaks, ω_p, are determined by zeros in Re(ϵ)
2. We fit a sum of loss functions at q=0:

This methodology is only a proxy for the true (unknown) q dependence. A more complete DFT or experimental analysis is required for any materials of interest

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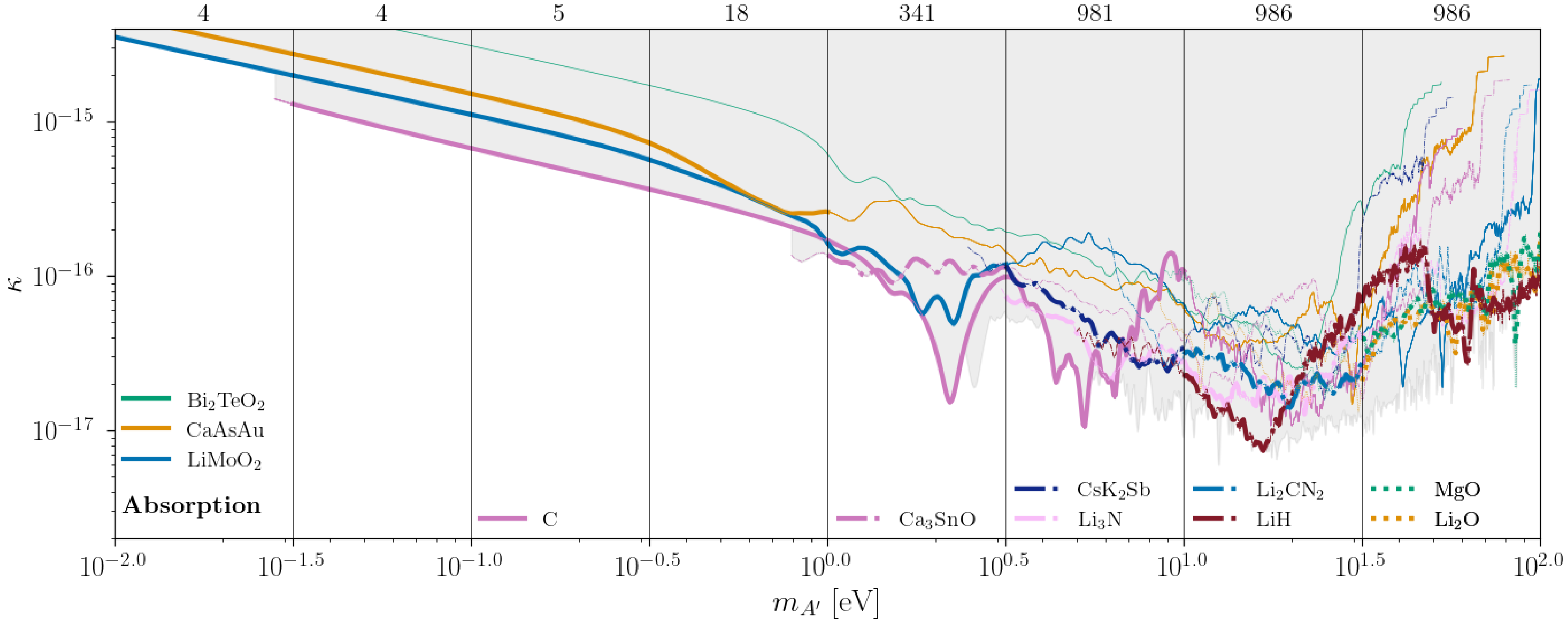
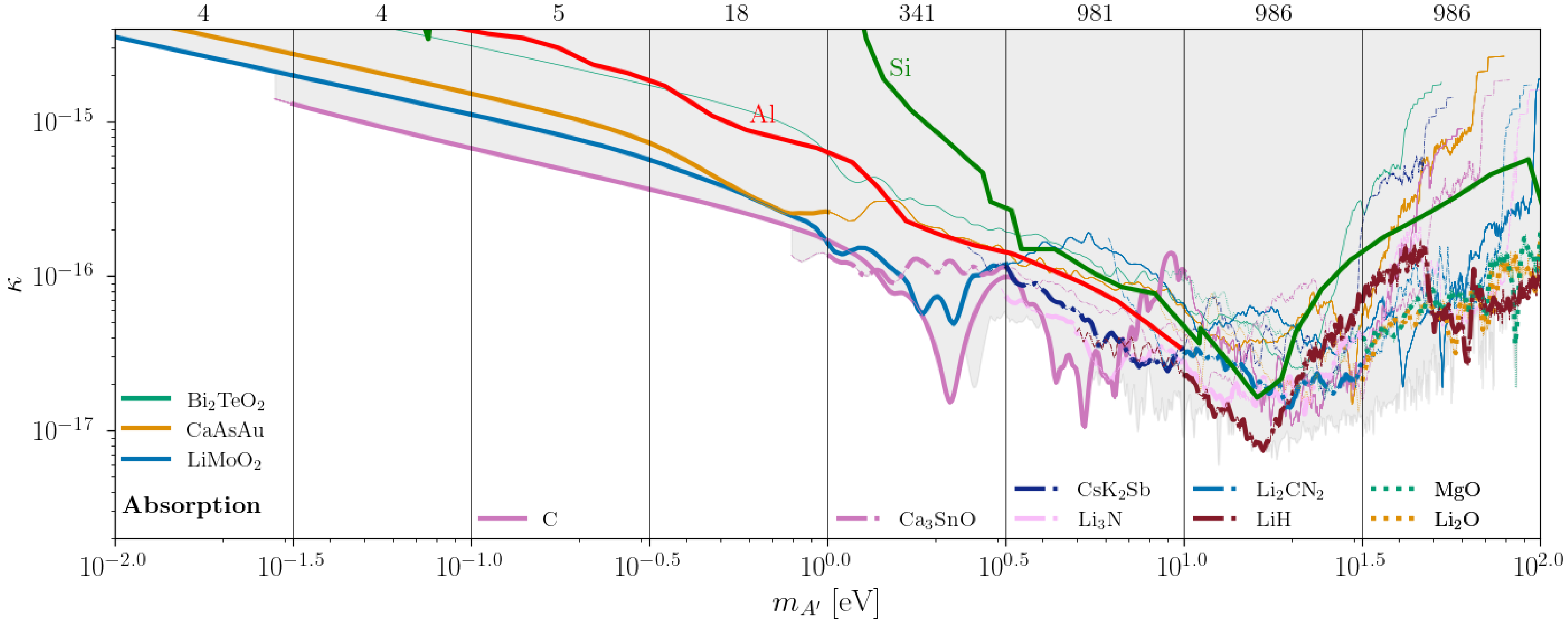
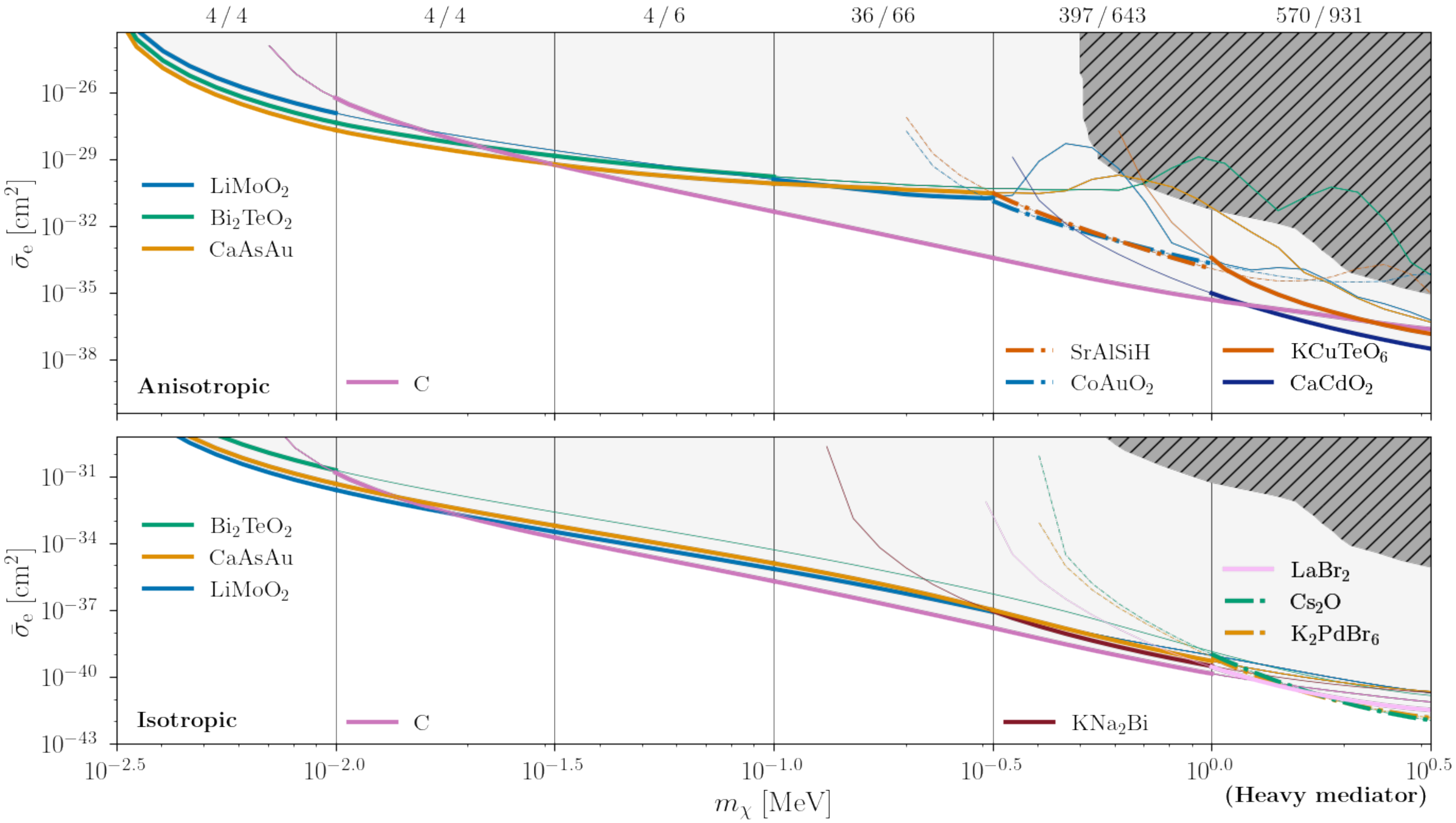
Absorption


4
4
5
18
341
981
986
986
10^{-15}
10^{-16}
10^{-17}
κ
Bi_2TeO_2
CaAsAu
$LiMoO_2$
Absorption
C
Ca_3SnO
CsK_2Sb
Li_3N
Li_2CN_2
LiH
MgO
Li_2O
$10^{-2.0}$
$10^{-1.5}$
$10^{-1.0}$
$10^{-0.5}$
$10^{0.0}$
$10^{0.5}$
$10^{1.0}$
$10^{1.5}$
$10^{2.0}$
$m_{A'}$ [eV]

Absorption

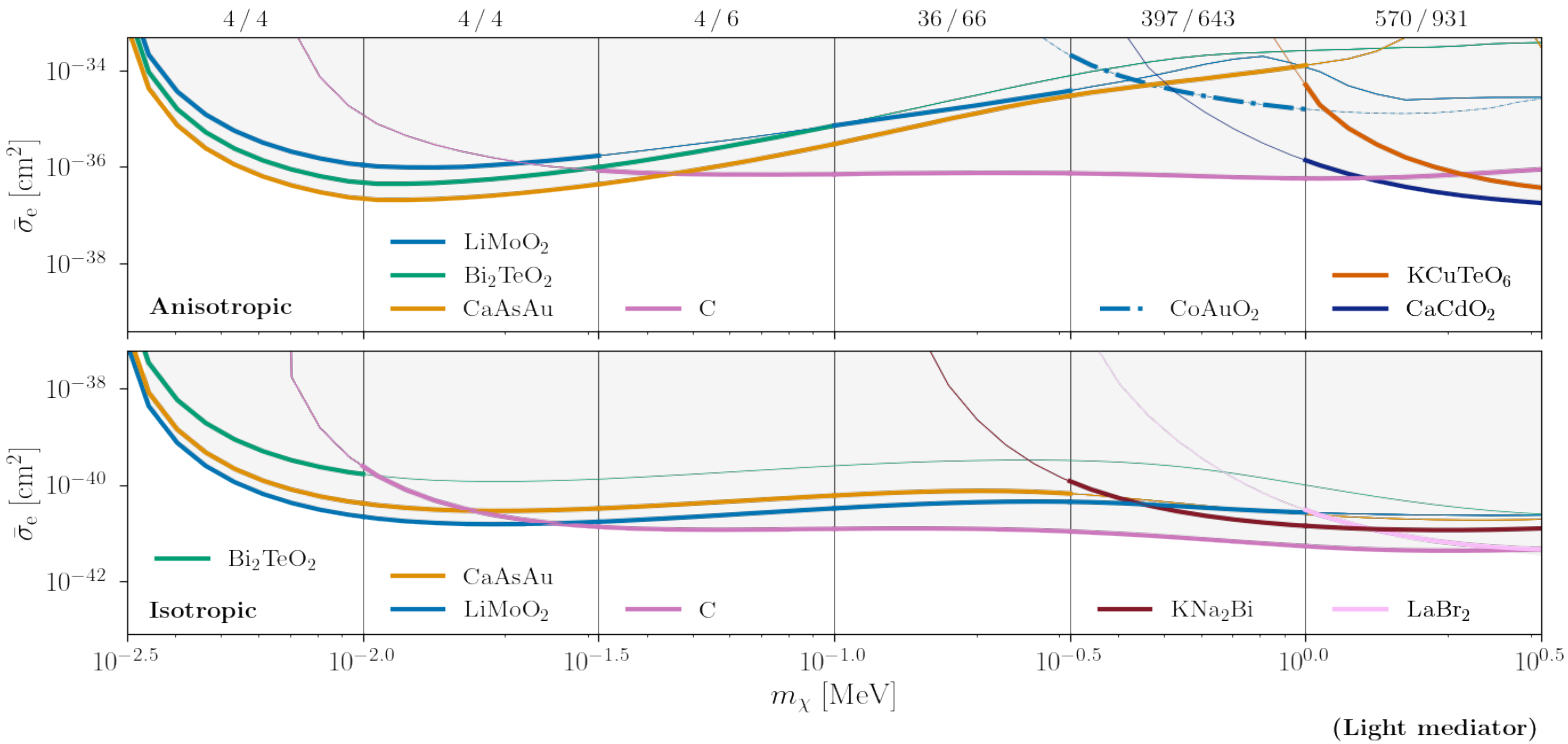

4
4
5
18
341
981
986
986
Si
Al
10^{-15}
10^{-16}
10^{-17}
κ
Bi_2TeO_2
CaAsAu
$LiMoO_2$
Absorption
C
Ca_3SnO
CsK_2Sb
Li_3N
Li_2CN_2
LiH
MgO
Li_2O
$10^{-2.0}$
$10^{-1.5}$
$10^{-1.0}$
$10^{-0.5}$
$10^{0.0}$
$10^{0.5}$
$10^{1.0}$
$10^{1.5}$
$10^{2.0}$
$m_{A'}$ [eV]

Heavy Mediator



$E_{th} = 10\ meV$

Light Mediator



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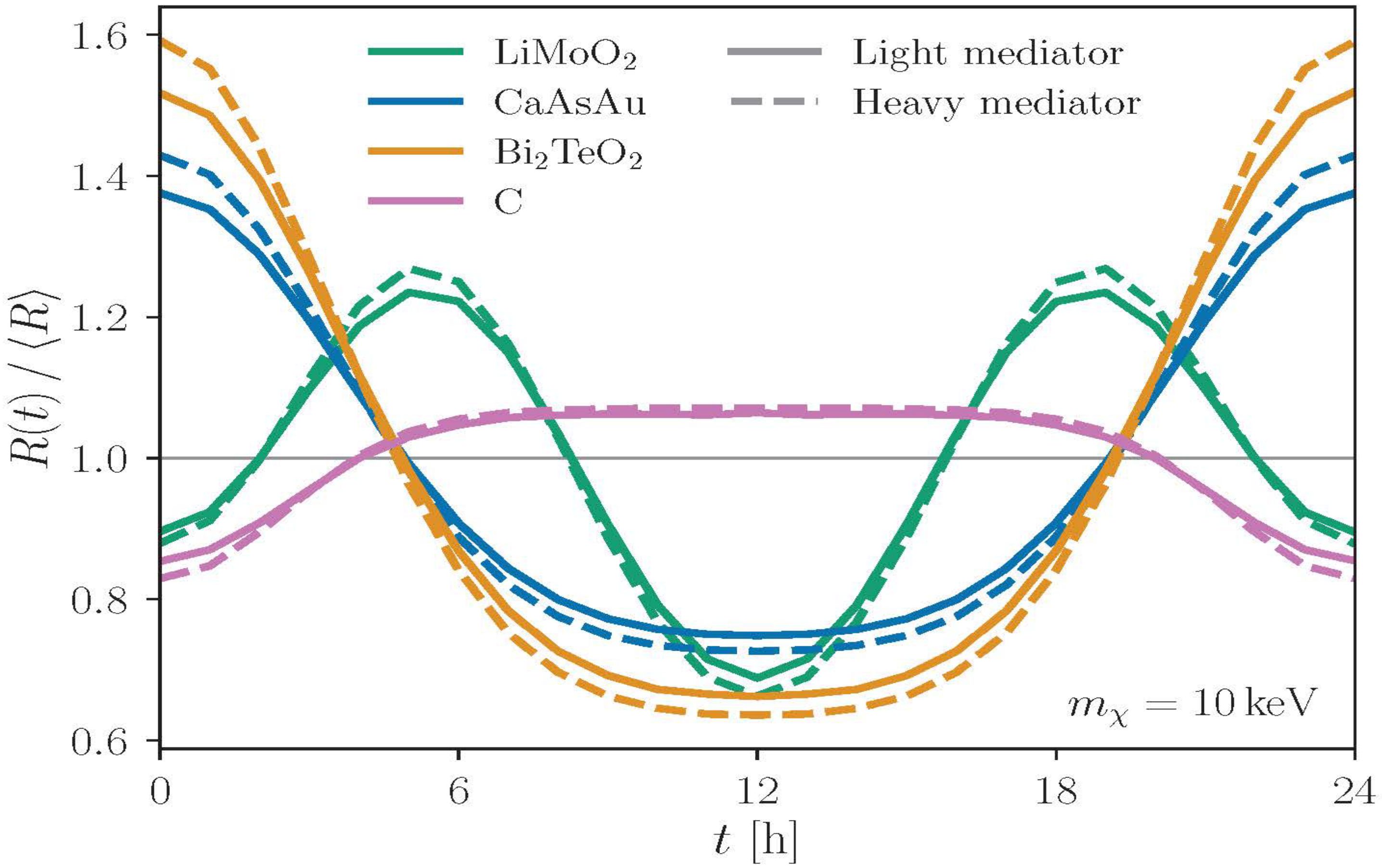
Daily Modulation



Our Dataset

- 1019 Materials with DFT computed, energy dependent, dielectric tensors
- 593 materials have anisotropic responses in at least 1 axis
  - We can do both an isotropic and anisotropic scattering analysis
  - Anisotropic scattering eliminates the background for a streaming DM signal, at the cost of requiring more DM interactions.
- Calculated in the limit of transferred momentum q -> 0
  - Scattering rate calculation requires q ≠ 0 data 😞