First High-Throughput Search for Dark Matter Detector Materials

BETHANY SUTER | UC BERKELEY

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IN COLLABORATION WITH YONIT HOCHBERG, BENJAMIN LEHMANN, ROTEM OVADIA, SINEAD GRIFFIN, RUO XI YANG, & WAYNE ZHAO





Outline





Materials Project & Big Data





Outline

Motivation of DM-Electron Scattering



Materials Project & Big Data



Kinematic Matching: Nuclear Recoil



Kinematic Matching

Light DM



Kinematic Matching: Electron-DM

Light DM

Electron



Electronic Screening: DM

Light DM



Electronic Screening: Dielectric Function



Electronic Screening: Dielectric Function



DM-Electron Scattering Rate



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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.

Our Dataset

- 1019 Materials with DFT computed, energy dependent, dielectric tensors
- 295 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 $q \neq 0$ data \bigotimes

How to Extract Momentum Dependence

• The Lindhard Dielectric Function has momentum dependence:

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

• Derived using perturbation theory and the Random Phase Approximation (RPA)

Models materials with one plasmon peak very well

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

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

 k_f , v_f can be derived from ω_p

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

Fitting Difficult Dielectric Functions



Full Pipeline

- 1. Locations of peaks, ω_p , are determined by zeros in Re(ϵ)
- 2. We fit a sum of Lindhards 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

features not described by Lindhard plasmons are independent of q

4. We calculate the scattering rate using $\epsilon(q, \omega) = r(\omega) \epsilon_{fit}(q, \omega)$

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

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Absorption



Light Mediator



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Heavy Mediator



 $E_{th} = 1 \ eV$

Conclusions

We've performed the first high throughput search for optimal materials with which to search for dark matter via direct detection

We utilized a model of the electron – DM scattering rate which correctly accounts for electron screening and depends on the particular material's dielectric function

We took dielectric tensor data from the Materials Project and modeled each material via a sum of Lindhard dielectric functions in order to approximate momentum dependence

We show the top three materials in many energy bands for absorption, and scattering with both heavy and light mediators.



Happy Birthday Hitoshi