



Contribution ID: 261

Type: **Poster presentation**

Density functional theory guides the search for dark matter particles in direct detection experiments

Tuesday 19 July 2022 19:00 (1 hour)

We use a combination of density functional and effective field theories to calculate the electronic structure of materials that are promising detectors for light dark matter and to predict the corresponding signal rates. Since light dark matter particles are more likely to interact with electrons in materials than to kinematically excite the atomic nuclei that were the focus of searches to date, an accurate description of the detector material's electronic structure is essential. Density functional theory provides such a description through explicit solution of the many-body Schrödinger equation, within a mean-field treatment of the inter-electronic exchange and correlations. We present calculated scattering rates for dark matter – electron scattering in existing semiconductor detectors, allowing us to exclude some regions of possible dark-matter phase space, and explore carbon-based materials for possible future detectors.

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