

First-principles screening of mineral candidates for dark matter detection with the PALEOCCENE technique

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At the lowest threshold for particle detection using the PALEOCCENE technique, nuclear recoils may result in only small numbers of single vacancy or interstitial defects. When such defects are optically active color centers, they can be used to image damage tracks down to atomic-scale resolution. First principles calculations are an effective approach for screening large numbers of minerals based on their propensity to form color centers from nuclear recoils. We begin by describing the methodology for calculating the electronic and optical properties of color centers, showing how careful tuning of the hybrid functional to simultaneously satisfy the generalized Koopman's theorem and reproduce the experimental band gap, enables precise prediction of emission wavelengths and formation energies. We demonstrate the accuracy of this method by comparing with experimental results in lithium fluoride. Finally, we conclude by showing how this method can be used to screen candidate materials for mineral detection of dark matter, and identify systems where single vacancy and interstitial defects are stable, optically bright color centers.

Do you plan to give the talk in person?

Yes

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