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Color center defect optical properties and formation dynamics across mineral candidates for dark matter detection

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The presence of color center defects in ancient minerals can be used to infer rare, high-energy nuclear recoil events due to neutrinos and dark matter. In order to be suitable for this approach, a mineral needs to have a propensity to form optically active color center defects as a result of lattice damage and subsequent relaxation. First-principles methods for computing electronic and optical properties have been very successful in explaining the behavior of color center defects for quantum applications in silicon, diamond, and other pristine, non-polar materials. However, accurate prediction of defect properties in natural minerals such as halite, olivine, and corundum pose a challenge for ab initio methods, due to their polar structures, complex compositions, and disorder. We overview the various computational approaches used to predict optical properties and formation of color center defects in minerals, including the selection of hybrid functionals to reproduce experimental optical transitions [1,2], charge and spin state effects on formation energies and barriers, and configurational averaging to account for lattice disorder. We present recent results on promising mineral candidates and discuss their suitability for detecting nuclear recoil events.

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[1] Gabriela A. Araujo, Laura Baudis, Nathaniel Bowden, Jordan Chapman, Anna Erickson, Mariano Guerrero Perez, Adam A. Hecht, Samuel C. Hedges, Patrick Huber, Vsevolod Ivanov, Igor Jovanovic, Giti A. Khodaparast, Brenden A. Magill, Jose Maria Mateos, Maverick Morrison, Nicholas W. G. Smith, Patrick Stengel, Stuti Surani, Nikita Vladimirov, Keegan Walkup, Christian Wittweg, Xianyi Zhang. "Nuclear recoil detection with color centers in bulk lithium fluoride." arXiv:2503.20732 (2025).

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