AB INITIO PROPERTIES OF COLOR CENTER DEFECTS FOR MINERAL DETECTION OF DARK MATTER. Pranshu Bhaumik, Tatsu Takeuchi & Vsevolod Ivanov, Dept. of Phys., Va. Polytechnic Inst. & State Univ. The existence of dark matter is strongly motivated by decades of astronomical measurements of its gravitational influence across a variety of scales, which have constrained its properties as stable over billions of years, electromagnetically non-interacting, and produced at low velocities. No known particles have these exact properties, making the detection and study of dark matter an essential part of developing particle physics beyond the Standard Model. Many existing theories predict dark matter to weakly interact with ordinary matter through nuclear recoils that generate detectable scintillation light or phonons. Experimental efforts to detect dark matter based on these effects are limited by target masses on the order of tons and observational timescales of years, making the detection of low-probability nuclear recoil events challenging. Instead, one proposal to improve detection involves using optically active point defects formed through nuclear recoils over millions of years in ancient deposits of common crystalline minerals such as fluorspar and calcium fluoride. Here, we perform ab initio simulations of simple defects in calcium fluoride, including interstitials and vacancies, and analyze their electronic and optical properties. We discuss how these potential signatures of nuclear recoils might be observed in fluorspar used for mineral detection of dark matter. Author contact: [vivanov@vt.edu](mailto:vivanov@vt.edu).