FIRST PRINCIPLES SIMULATION OF COLOR-CENTER DEFECTS IN LITHIUM FLUORIDE FOR SENSING LOW-ENERGY NUCLEAR RECOILS. Mariano Guerrero-Perez, Tatsu Takeuchi & Vsevolod Ivanov, Dept. of Phys., Va Polytechnic Inst. & State Univ. Despite mounting evidence from gravitational anomalies in astronomical measurements of stars, galaxies, and the cosmic microwave background suggesting dark matter accounts for 85% of matter in the universe, dark matter particles have yet to be observed directly. The current data is in favor of low-velocity “cold” dark matter which weakly interacts with conventional matter, resulting in nuclear recoils that produce scintillation light or phonons detectable using large quantities of cryogenic crystals or liquefied noble gasses. As an alternative sensing method, it has been suggested that next-generation dark matter experiments might instead look for photons emitted from color-center defects generated by nuclear recoils. Materials used for this kind of approach would need to be cost effective, optically transparent, and readily generate bright color center defects from nuclear recoils. Here we use first principles methods to model one such candidate material, lithium fluoride, and predict the properties of simple color center defects. We consider lithium and fluorine interstitials and vacancies, computing formation energies, charge states. emission frequencies, brightness, and radiative lifetimes, and discuss the potential of using lithium fluoride crystals for directional detection of dark matter and other particles. (Supported by: The Inclusive Excellence project at Va. Polytechnic Inst. & State Univ. (https://ie.vt.edu/), based on a grant from the Howard Hughes Medical Institute.) Author contact: [vivanov@vt.edu](mailto:vivanov@vt.edu).