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Thorium-229 solid-state nuclear clock prospects in MgF_2 and LiSAF EDMUND MEYER, BEAU BARKER, LEE COLLINS, Los Alamos National Laboratory — The ^{229}Th isomer is thought to be a good candidate for a nuclear clock based on its relatively low-energy isomer excitation of $\approx$ 7.8 eV. We report on the study of Th atoms embedded in two crystals, MgF_2 and LiSAF ($LiSrAlF_6$). For MgF_2 we perform an oxidation study to find the preferred ionization state of the Th atom in the crystal; Th^{n+}, where $n = 2-4$. We find that the preferred state is $n = 4$ which requires two interstitial Fluorine atoms to charge compensate. Using the results of MgF_2 we then search within LiSAF for suitable dopant sites (the Sr, Al, or Li can all serve). Employing a standard density functional package using a plane-wave basis and psuedopotentials, we optimize a doped cell of increasing particle number sizes and use this to estimate the dilute doped-limit band-gap of LiSAF. Placement of the dopant on the Sr and Al sites with accompanying double and single F interstitial atom placements is also studied to determine the ground state, and comparisons are made with previous calculations [1]. In both crystal ground states, we find that the band gap is large enough for the observation of the ^{229}Th nuclear isomer transition; > 9 eV.
[1] R. A. Jackson et al., J. Phys.: Condens. Matter 21, 325401 (2009).

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