

PAW study of the F-center in LiF¹
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One of the earliest and most extensively studied defects in ionic solids is the F-center, which results from replacement of an anion with a single electron. The RMS radius of the F-center can be calculated from optical spectra using the Vinti sum rule, and has been calculated for many alkali halides². In the alkali halides, this radius is found to vary linearly with the lattice constant of the host crystal. In this work, we used the projector augmented wave code^{3,4,5} (PAW) to determine the F-center wave function. Like the pseudopotential approach, the PAW method performs all calculations using smooth wave functions, but is able to recover the full nodal wave functions of the all-electron Hamiltonian. Thus, we are able to calculate the RMS radius of the F-center from first principles. Using a 15-atom unit cell, periodic boundary conditions, and the local density approximation, we determine the RMS radius of the F-center in LiF to be 2.1 Å, compared to the value of 1.5 Å found from optical spectra.²

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