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Electronic Structure Calculations of Iron-doped Zinc Selenide[1]
EVAN GARRISON, KYLE BENTLEY, RYOICHI KAWAI, Department of Physics, The University of Alabama at Birmingham — II-VI semiconductors doped with transition metal ions are good candidates for mid-infrared laser materials. Among them, iron-doped zinc selenide (Fe:ZnSe) appears to be one of the most promising. However, its detailed properties are still not well understood. We have investigated the electronic and geometric structures around the Fe ion dopant in ZnSe using density functional theory. The geometry around substitutional and interstitial dopants are fully optimized using a large supercell consisting of 217 atoms. First, we confirmed that Fe^{2+} with quintet spin (S=2) is the most stable state. The lattice distortion around the dopant is found to be very small. We identified two electronic orbits inside the band gap which are used in the laser application. We found the excitation energy to be 0.329 eV, consistent with the experimental data. The upper state is very close to the conduction band, suggesting that the excited electron may go to the conduction band.

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