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Crystal structure prediction of Fe_3Se_4 using the evolutionary algorithm coupled with first principles DFT simulations NABIL AL-AQTASH, RENAT SABIRIANOV, University of Nebraska at Omaha — The evolutionary algorithm coupled with the first-principles Density Functional Theory (DFT) method is used to identify the global energy minimum structure of Fe_3Se_4. The structure is processed by free-energy based evolutionary crystal structure optimization algorithms, as implemented USPEX and XtalOpt codes, which predict structure of the system solely based on the chemical formula without prior experimental information. This is very challenging task for verifying the validity of this approach on Fe_3Se_4 structure. Fe_3Se_4 has highly anisotropic structure, and its structure demonstrates ordering of vacancies that makes the system "open", i.e. breaking traditional coordination rules. By using USPEX and XtalOpt we identify the global minimum of Fe_3Se_4 structure. The randomly generated initial population had 20 structures. The enthalpy (tolerance of 0.002 eV), and space group were used for niching. The enthalpy of the lowest energy structure, out of 700 generated structures that were generated, is (-81.126 eV). Bulk Fe_3Se_4 has a monoclinic structure with a space group of *I2/m* and $a = 6.208$Å, $b = 3.541$Å, and $c = 11.281$Å. The crystal structure and the lattice parameters of Fe_3Se_4 optimized from our calculations are similar to the experimental existing structure parameters. Fe_3Se_4 exhibits large magnetocrystalline anisotropy of $6x10^6$ erg/cm^3 and coercivity up to 40kOe due to its unusual properties.

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