Abstract Submitted for the MAR14 Meeting of The American Physical Society

Crystal structure prediction of Fe$_3$Se$_4$ 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$_3$Se$_4$. 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$_3$Se$_4$ structure. Fe$_3$Se$_4$ 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$_3$Se$_4$ 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$_3$Se$_4$ has a monoclinic structure with a space group of $I2/m$ and $a = 6.208\,\text{Å}$, $b = 3.541\,\text{Å}$, and $c = 11.281\,\text{Å}$. The crystal structure and the lattice parameters of Fe$_3$Se$_4$ optimized from our calculations are similar to the experimental existing structure parameters. Fe$_3$Se$_4$ exhibits large magnetocrystalline anisotropy of $6 \times 10^6 \,\text{erg/cm}^3$ and coercivity up to $40\,\text{kOe}$ due to its unusual properties.

Nabil Al-Aqtash
University of Nebraska at Omaha

Date submitted: 14 Nov 2013

Electronic form version 1.4