Fully-optimized study of the electronic structure of FeSe

Alex Koufos and D.A. Papaconstantopoulos
SPACS, George Mason University

We have performed density functional theory (DFT) calculations using the linearized augmented plane wave method (LAPW) with both the generalized gradient approximation (GGA) and local density approximation (LDA) functionals, to study the electronic structure of the iron-based superconductor, Iron-Selenium (FeSe). In our study, we have performed a most comprehensive set of calculations involving structural, atomic and spin configurations. All calculations were performed using the tetragonal lead-oxide (tetra-PbO) structure, with various volumes, c/a ratios and internal parameters. Furthermore, we investigated the spin polarization using the LDA and GGA to assess ferromagnetism in this material. The GGA calculations find the equilibrium configuration of FeSe for the tetra-PbO structure to have a volume of ~576au^3 with a c/a ratio of 1.70 and internal parameter of 0.22, with the ferromagnetic having slightly lower energy than the paramagnetic. For LDA, the equilibrium configuration for FeSe for the tetra-PbO structure is found to have a volume of ~464au^3 with a c/a ratio of 1.50 and internal parameter of 0.26, with the ferromagnetic also having slightly lower energy than the paramagnetic. In addition, we have started fitting the LAPW results on a tight-binding (TB) basis and obtained indications that the resulting TB Hamiltonian will be robust to use for applications such as molecular dynamics, vacancy formation energies, and even exploring properties beyond the DFT capabilities.