Electronic structure effects of FeV at high pressure

Homero Reyes Pulido and Jorge Muñoz
Physics Department, University of Texas at El Paso
500 W. University, El Paso, Texas 79968, USA
hreyes9@miners.utep.edu, jamunoz@utep.edu

Quantum mechanics is one of the most successful theories developed by mankind. However, to obtain analytical results from it is, in practice, complicated and not always possible. Density functional theory (DFT) has shown to be a reliable and affordable computational method for material analysis with great accordance compared with experimental data that has allowed deeper understanding of microscopic phenomena. To show this, we analyze the dynamical stability of the B2 phase of the equiatomic iron-vanadium (FeV) alloy to obtain a comprehensive explanation of the increase in anharmonicity of certain phonon modes. The electron density of states (eDos) is calculated to observe the behavior of the eg and t2g orbitals to help us describe the electron transfer occurring at different volumes. The band structure for both spin-up and spin-down of our results is also computed to analyze the differences in the structure close to the Fermi energy. A clear change in the plots suggest a strong magnetization loss due to phonon-electron interaction.