Abstract Submitted
for the TSS21 Meeting of
The American Physical Society

Electronic structure effects on the phase stability of B2 FeV HOMERO REYES , JORGE MUOZ, University of Texas at El Paso — Recently we predicted, using classical molecular dynamics, that a known dynamical instability in the BCC-based B2 phase of the alloy iron-vanadium (FeV) at 0 K disappears at elevated temperature due to phonon anharmonicity. In this talk we will present density functional theory (DFT) results that elucidate the causes at the electronic structure level. First, we study the effects of pressure on a 2-atom cell of B2 FeV. The momentum-projected density of states (eDOS) is calculated and the charge in the e_g and t_2g $orbitals$ is $extracted$ $upon$ $compression.$ The $band$ $structure$ for $both$ $spin-up$ and $spin-down$ is $computed$ and a $change$ is $observed$ at the X and $high$ $symmetry$ $points$ $upon$ $compression.$ $Second,$ we use $Oppenheimer$ $molecular$ $dynamics$ to $investigate$ a 16-$atom$ $supercell$ of FeV and $both$ the $momentum-projected$ $eDOS$ and the $charge$ in the e_g and t_2g $orbitals$ as a $function$ of $temperature$ $were$ $calculated.$ The $value$

Homero Reyes
University of Texas at El Paso

Date submitted: 11 Mar 2021 Electronic form version 1.4