Atomic modeling of stability and thermal characteristics of metastable tungsten as a plasma-facing fusion material\(^1\) ANNA WOLZ, University of Virginia, JEROME GUTERL, Oak Ridge Associated Universities, STEFAN BRINGUIER, General Atomics — Plasma-facing materials must be able to sustain large heat and particle fluxes in future fusion reactors. Recent experiments have suggested the existence of a metastable W-B phase at room temperature \([1]\) which may be a suitable plasma-facing material. Exploring the influence of implanted species on lattice stability and thermal properties therefore provides additional insight. First, the stability of W phases BCC and FCC is analyzed by solving the phonon dispersion relation at various temperatures (0-4000K) and pressures (100-105 atm). The phonon spectra are deduced from the eigenvalues of the dynamical matrix obtained from molecular dynamics simulations (LAMMPS) \([2]\), and compared to existing calculations for pure W \([3]\) to assess the validity of the phonon calculation and interatomic potential. The effects of impurities on the stability of W phases are examined from the phonon spectra when H, He, and B impurities are introduced into a W lattice. \([1]\) Y. Raitses, 60th APS-DPP conference 2018 \([2]\) Zhang, H. Y (2018). Computational Materials Science, 144, 32-35 \([3]\) Kong, L. T. (2011). Computer Physics Communications, 182(10)

\(^1\)Work supported in part by US DoE under the Science Undergraduate Laboratory Internship (SULI) program and under DE-SC0018423, DE-FC02-04ER54698 and DE-FG02-91-ER54109