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Elastic Constants and Phonons of Tungsten-Nitride from First Principles CHRISTIAN DANE, DANIEL FINKENSTADT, U.S. Naval Academy, MICHAEL MEHL, Naval Research Laboratory, STEFANO CURTAROLO, Duke University — Certain Tungsten Nitride (WN) crystal structures have been found to exhibit tendencies for exceptional hardness. Some researchers [S. Aydin et al., J. Mater. Res. 27, 1705 (2012)] have made the claim that these structures have hardness qualities that rival diamond. There are three specific structures with unique compositions that are of interest. By calculating the bulk and shear moduli as well as analyzing phonon dispersion plots, the properties of these structures can be compared to known structures like diamond. We used VASP density-functional methods implemented within the MedeA software package to strain each structure in a series of directions in increasing amounts. A simple linear fit of stress vs. strain found that the leading structure in terms of thermodynamic stability has elastic constants of C_{11} = 753 GPa, C_{12} = 126 GPa, and C_{44} = 172 GPa. These constants, while high, are significantly lower than diamond's. This indicates that previous calculations may have been mistaken in predicting the qualities of the WN system. Some of the difference between our results is due to the exchange-correlation functional chosen, namely, LDA vs. GGA.

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