

Abstract Submitted  
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**First-Principles Calculation of forces and phonons in solid** ZHENHUA NING, WILLIAM SHELTON, Louisiana State University — We have developed a multiple scattering theory approach to calculate Hellmann-Feynman forces and phonons via the calculation of the force constant and dynamical matrix. To demonstrate the accuracy and validity of our approach we compare with the ELK code, which is a full potential Linear Augmented Plane Wave (FLAPW) based method. As we will show our forces and phonon dispersion curves are in good agreement with the FLAPW code. This work lays the foundation for developing a first principles approach for calculation of phonons in substitutionally disordered materials.

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