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Computational investigations of mechanical and dynamical properties of gold-based compounds (X₃Au, X=Ti, Zr and V)

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Highlights

- Elastically, X₃Au (X=Ti, Zr and V) compounds were found to be mechanically stable.
- X₃Au compounds are ductile in nature.
- \bullet The phonon spectra of X_3Au compounds revealed that they are dynamically stable in the A15 structure.



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