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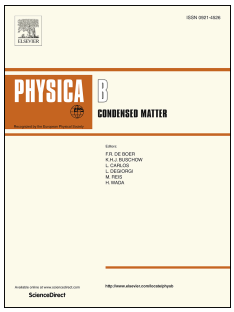

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Ab initio study of structural, elastic, and vibrational properties of transition-metal disilicides $NbSi_2$ and $TaSi_2$ in hexagonal C40 structure

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Abstract

We present an *ab initio* study of structural, elastic and vibrational properties of transition-metal disilicides $NbSi_2$ and $TaSi_2$. The calculations have been carried out within the density-functional theory and linear-response formalism using norm-conserving pseudopotentials and a plane-wave basis. The calculated lattice parameters, bulk moduli, and elastic constants agree well with previous theoretical and experimental results. The calculated phonon frequencies at the Brillouin zone center are in good agreement with the reported Raman spectra and provide reference values for the future infrared and neutron phonon measurements. Phonon dispersion relations, mode Grüneisen parameters, and total and partial phonon density of states are also discussed. Mode Grüneisen parameters of $NbSi_2$ and $TaSi_2$ at Brillouin zone center show similar trends and all values are found to be positive. From phonon dispersion relations and phonon density of states, we have found a gap around 200 cm^{-1} for $TaSi_2$, where the frequencies below this gap mainly belong to Ta vibrations and frequencies above the gap is mainly related with Si vibrations. In the case of $NbSi_2$, there is no such gap and both Nb and Si atoms contribute to the phonon density of states in an energy range of 150-270 cm^{-1}.

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