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Computational modelling studies of Pd tellurides

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Abstract content
   (Max 300 words)
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Telluride minerals are minor or trace components in ore deposits from a wide variety of geological environments. They are also important carriers of precious metals, especially of Pt, Pd, Au and Ag. In nature, tellurides of palladium are most widely spread. Metal tellurides are applicable mainly in optical devices such as solar cells, but also in thermoelectrical devices. Density functional theory study is used to investigate structural stability in terms of heats of formation, elastic constants and phonon dispersion for the PdTe, PdTe₂ and Pd₃ Te₂ structures. In order to investigate the mechanical stability, we evaluated their phonon dispersion curves along symmetry direction within the first Brillouin zones. The elastic properties of the PdTe, PdTe₂, and Pd₃, Te₂ satisfied all necessary conditions for mechanical stability. Thus, all the systems are predicted to be mechanically stable.

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