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Quantum mechanical ab initio calculations of the structural, electronic, vibrational, mechanical and optical properties of bulk Silicon tellurides

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Silicon tellurides are being considered for next-generation non-volatile memory material. For the applications of these materials in electronic devices, it is necessary to provide information on their thermodynamic and mechanical stabilities, structural, electronic and optical properties based on first-principles density-functional theory. The obtained results are compared with experiment and with some available previous calculations.

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