239
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Title:First-principles investigations on elastic, phonon and thermodynamic properties of SrB<inf>6</inf> under pressure
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Abstract:The elastic, phonon and thermodynamic properties of the divalent alkaline-earth hexaboride SrB<inf>6</inf> are investigated by using plane-wave pseudopotential density functional theory method. The calculated structure parameters and bulk modulus are well consistent with the available experiment and theoretical data. The pressure dependences of elastic constants C <inf>ij</inf>, bulk modulus B<inf>0</inf>, shear modulus G, Youngs modulus E and Poissons ratio σ are also presented. With these elastic parameters, we investigate the mechanical stability and compressibility of SrB<inf>6</inf>. For the thermodynamic properties, both phonon and quasi-harmonic Debye model methods are adopted. Through the comparison with experimental and other theoretical results, we found the method of quasi-harmonic Debye model is a little better. Moreover, the phonon dispersion relations are also obtained. It is found that there are two LO/TO splitting around 5 THz and 26 THz, respectively. 
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