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Electronic structural, optical and phonon lattice dynamical properties of pure- and La-doped $SrTiO_3$ YUHUA DUAN, PAUL OHODNICKI, BENJAMIN CHORPENING, Natl Energy Technology Lab — To better understand the thermodynamic and optical behaviors of lanthanum doped strontium titanate (LSTO) with different La-doping levels at high temperature, the *ab initio* thermodynamics by combining the first-principles density functional theory with lattice phonon dynamics have been employed to investigate their electronic structures and thermodynamic evolutions versus temperatures. The results show that when doping La into STO, the band-gap is vanished as extra electron fills into the STO conduction band. With increasing the La-doping levels, the LSTO structures become unstable with phonon soft modes. From the calculated dielectric constant matrix of LSTO with different La-doping levels, one can see that in three cases (2La-STO, 3La-STO, 6La-STO) their diagonal elements are not equal, which means that these crystal structures are uniaxial and anisotropic. With increasing La-doping levels, the calculated thermodynamic properties (ΔH, ΔG) with reference to DFT energy of pure STO are decreased. With increasing temperature (T), the ΔH(T) is increased while the ΔG(T) is decreased.

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