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Elastic, electronic, thermodynamic and transport properties of *X*OsSi (*X*=Nb, Ta) superconductors: First-principles calculations

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Abstract

First-principles calculations have been performed to study elastic, electronic, thermodynamic, transport and superconducting properties of recently reported osmium based two superconductors, *X*OsSi (*X*=Nb, Ta). We have calculated elastic constants and elastic moduli of *X*OsSi compounds for the first time. The calculated values of bulk, Young's, shear moduli are slightly larger than the average value obtained from the rule of mixtures of the constituents. NbOsSi and TaOsSi both compounds are found to be relatively hard material, elastically stable and ductile in nature. The obtained directional bulk modulus and shear anisotropic factors indicate that both compounds have high elastic anisotropy. The shear anisotropic factors show higher elastic anisotropy than the percentage anisotropy in these compounds. The Debye temperature and bulk modulus increases with pressure but decreases with temperature as usual for metals. The magnetic susceptibility (χ) of TaOsSi follows the Curie law but NaOsSi does not follow due to its delocalized magnetic moment and electronic specific heat (c) slightly deviates from the linear relationship with temperature. The calculated band structures of *X*OsSi compounds exhibit metallic nature. In both cases, d-orbitals have the dominating contribution to the total density of states. The smaller electron-phonon coupling constant implies that *X*OsSi (*X*=Nb, Ta) are weakly coupled superconductors.

Keywords: *X*OsSi (*X*=Nb, Ta); Elastic properties; Electronic properties; Thermodynamic properties; Transport properties; Superconductivity.