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Electronic, optical, elastic, thermoelectric and thermodynamic properties of the spinel oxides $ZnRh_2O_4$ and $CdRh_2O_4$

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Abstract

Density functional FP-LAPW+lo method calculations were performed to explore the structural, electronic, optical, elastic, thermoelectric and thermodynamic properties of the spinel oxides $ZnRh_2O_4$ and $CdRh_2O_4$. The exchange-correlation potential were described using the GGA-PBEsol and TB-mBJ functionals. As the first step, the optimized structural parameters, including the lattice parameter and atomic coordinates, were determined. Electronic band structure, atomic-resolved *l*-projected densities of electronic states and photon energy dependence of the linear optical functions were computed. It is found that both investigated compounds are indirect band gap semiconductors. The band gap results from the splitting of the $\mathrm{Rh}:4d^6$ states into occupied $\mathrm{Rh}:4d-t_{2g}^6$ states, which form the valence band maximum (VBM), and the empty states $\mathrm{Rh}:4d-e_g^0$, which form the conduction band minimum (CBM), owing to the octahedral substantial crystal-field. The electronic interband transitions responsible of the structures in the optical spectra were specified. Single-crystal and polycrystal elastic moduli, wave sound velocities, Debye temperature, Pugh's indicator and indexes of elastic anisotropy were numerically estimated using total energy versus strain. FP-LAPW+lo band structure in combination with the standard Boltzmann transport theory were employed to calculate the thermoelectric parameters, including Seebeck coefficient,