Highlights

- Using density functional theory (DFT), density functional perturbation theory (DFPT), and Boltzmann transport theory the electronic, phonon, and transport properties of ternary ZrS_xSe_{2-x} (x=0, 1, and 2) have been calculated.
- The p- doped $ZrSe_2$ has the highest power factor and the lowest bandgap between three compounds.
- The highest Seebeck coefficient is observed in ZrS_2.
- The lowest lattice thermal conductivity and the highest figure of merit (ZT) are found in ZrSeS.