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# Effect of pressure on structural, mechanical, dynamical and electronic properties of ReSe2 :A theoretical investigation

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Effect of pressure on structural, electronic, mechanical, and Dynamical properties of ReSe 2 has been investigated using the first-principles calculations.These calculations are based on density functional theory and were performed using the generalized gradient approximation with the empirical van der Waals correction. The calculated lattice parameters ReSe2 under effect of pressure are consistent with the available experimental values upto 9.03 GPa, which motivated us to explore the stated prperties beyond the 9.03 Gpa limit. The lattice parameters and volume of ReSe2 decrease with the increasing pressure whereas the total enthalpy increases. The mechanical properties are predicted using the Voigt–Reuss–Hill approximation from which there is an inverse relationship between volume and pressure implying that as we subject ReSe2 to large pressure the material becomes somehow more compact due to reduced inter-atomic distance hence increase in magnitude of elastic coefficients as well as bond strength. The Dynamical instability was investigated by computing the phonon frequency to check for imaginary modes. ReSe2 is dynamically stable below 40 GPa. The band gap was estimated using the Perdew-Burke-Ernzerhof (PBE) and modified Becke–Johnson potential, which confirmed that as pressure
increased, the band gap decreased in almost a linear manner.

## HPC content

We apply first-principles calculations based on density functional theory as implemented in VASP code. We use MPI to run our calculations with 24 and 72 cores usually, employing a 2x2x2 super cell (i.e 96 atoms for ReSe2), which is the problem size, the phonon dispersion is obtaining from the finite displacement method as implemented in the PHONOPY package. Using the same supercell we determine the lattice thermal conductivity using two methods. Firstly, a single-mode relaxation-time approximation as implemented in the PHONO3PY package. Secondly, an iterative self-consistent method with the ShengBTE code.

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