Effect of pressure on structural, mechanical, dynamical and electronic properties of $ReSe_2$: A theoretical investigation

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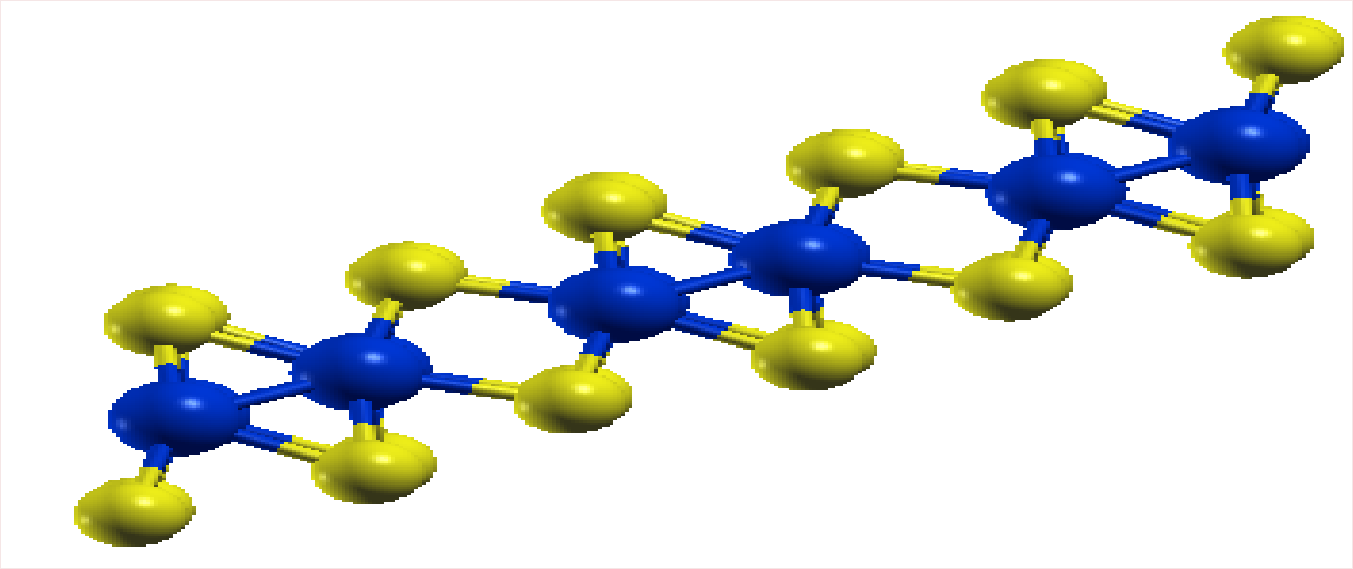
Outline

Introduction

- The study of the pressure and temperature phase diagram of semiconductors has continued for several decades now using powerful experimental techniques such as x-ray, neutron diffraction, and light scattering.
- Rhenium diselenides $ReSe_2$ belong to the family of layer-type transition metal dichalcogenides.



Computational Details

Structural and Electronic properties have been calculated by Density Functional Theory with the PBE and modified Becke Johnson potential (MBJ) using the VASP package

Phonon obtained from the finite displacement method as implemented in the PHONOPY package.

Equilibrium parameters $ReSe_2$

Lattice parameters	PBE[a]	$PBE+D3$	Expt[b]	Expt[c]
$a(\AA)$	6.67	6.82	6.60	6.72
$b(\AA)$	6.79	6.75	6.71	6.62
$c(\AA)$	7.76	6.71	6.72	6.73
$V(\AA^3)$	295.68	250.08	247.34	
$E_{coh}(eV)$	-4.72	-5.01		

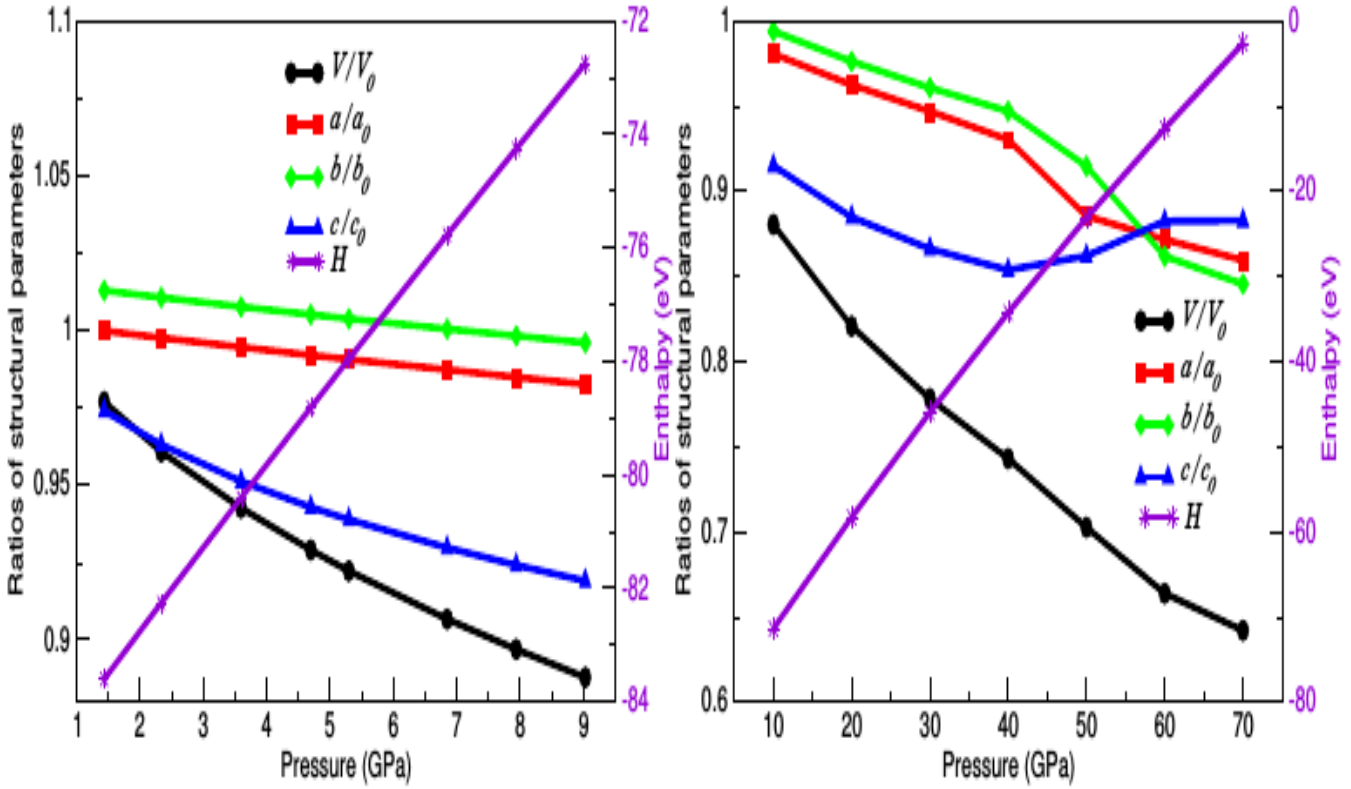
[a] Guy Moıse Dongho. Diss. University of the Witwatersrand, Johannesburg, 2016.
[b] J. Wildervanck and F. Jellinek. Journal of the Less Common Metals. 24. 73–81, 1971.
[c] W. Jeitschko and R. Rühl. Structural Crystallography and Crystal Chemistry. 35. 1953–1958, 1979.

Equilibrium parameters

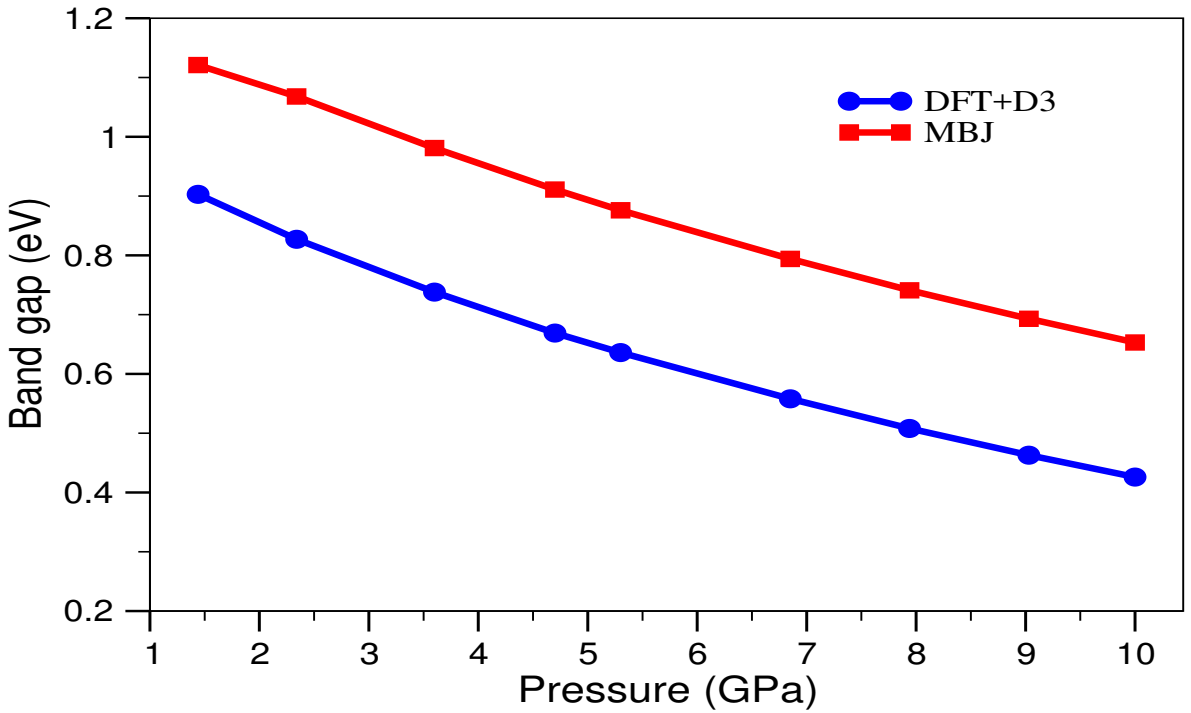
P (GPa)	Calcualtions				Experimental			
	$a(\AA)$	$b(\AA)$	$c(\AA)$	$V(\AA^3)$	$a(\AA)$	$b(\AA)$	$c(\AA)$	$V(\AA^3)$
1.44	6.599	6.796	6.545	241.63	6.585	6.698	6.584	241.02
2.34	6.584	6.781	6.472	237.63	6.565	6.677	6.508	236.70
3.60	6.564	6.761	6.392	233.14	6.543	6.659	6.446	232.95
4.70	6.547	6.744	6.336	229.79	6.523	6.636	6.373	228.80
5.30	6.538	6.735	6.309	228.11	6.519	6.633	6.351	227.72
6.85	6.516	6.713	6.248	224.26	6.503	6.615	6.286	224.20
7.94	6.500	6.698	6.210	221.84	6.495	6.606	6.253	222.36
9.03	6.485	6.683	6.176	219.60	6.492	6.604	6.224	221.06

Kao, Yu-Cheng, et al. 2 024509 2012.

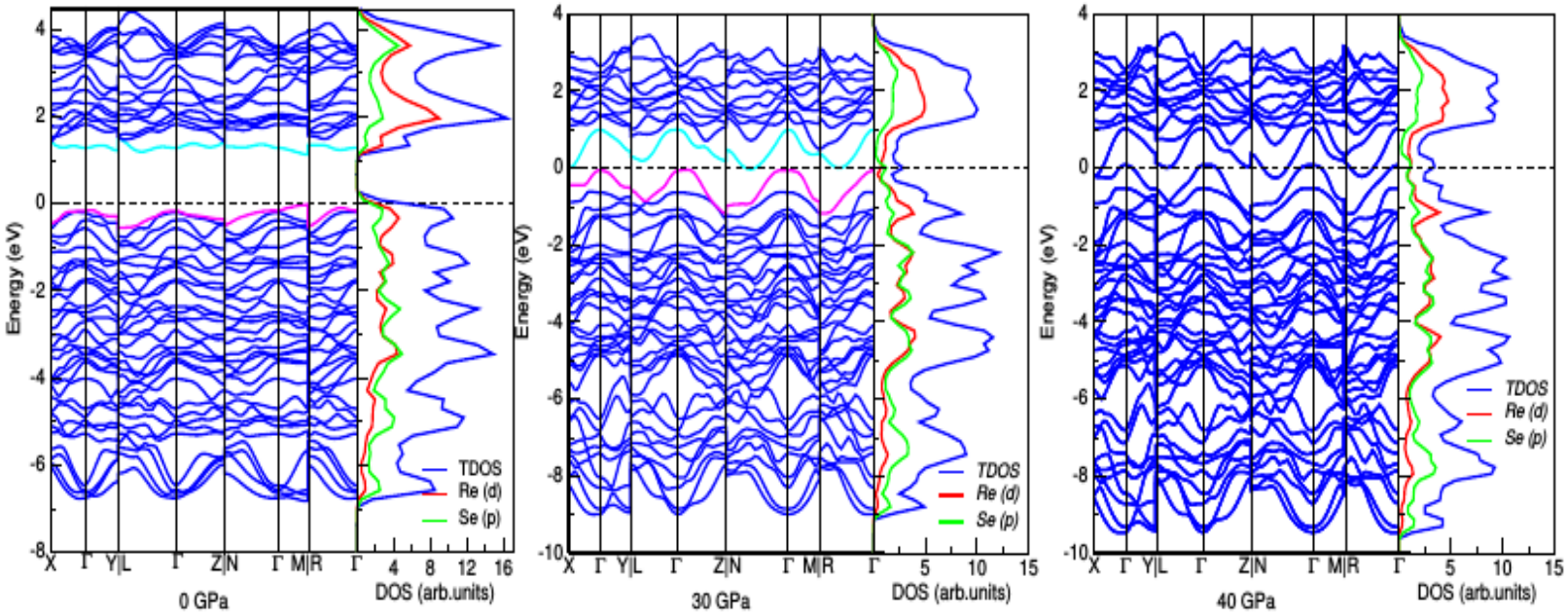
Equilibrium parameters



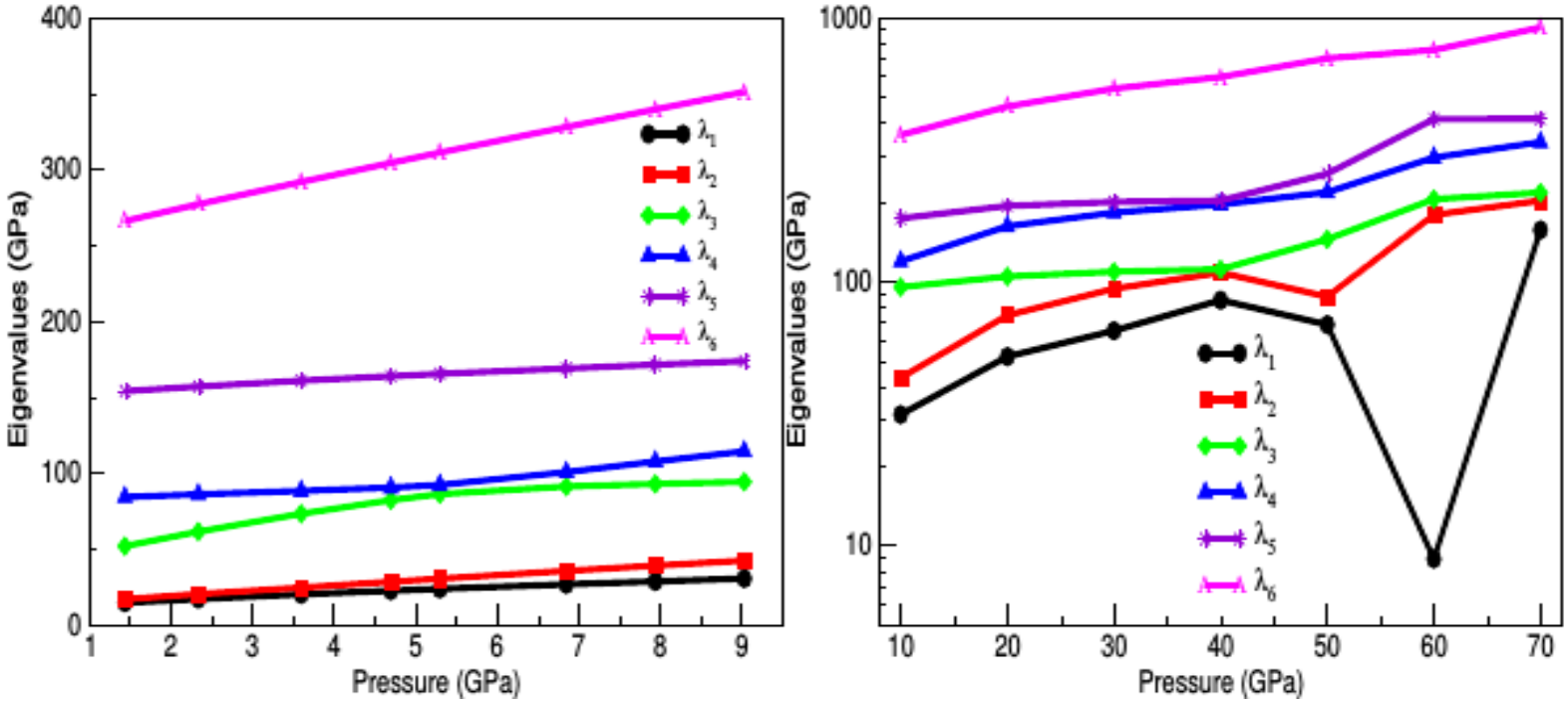
Electronic properties



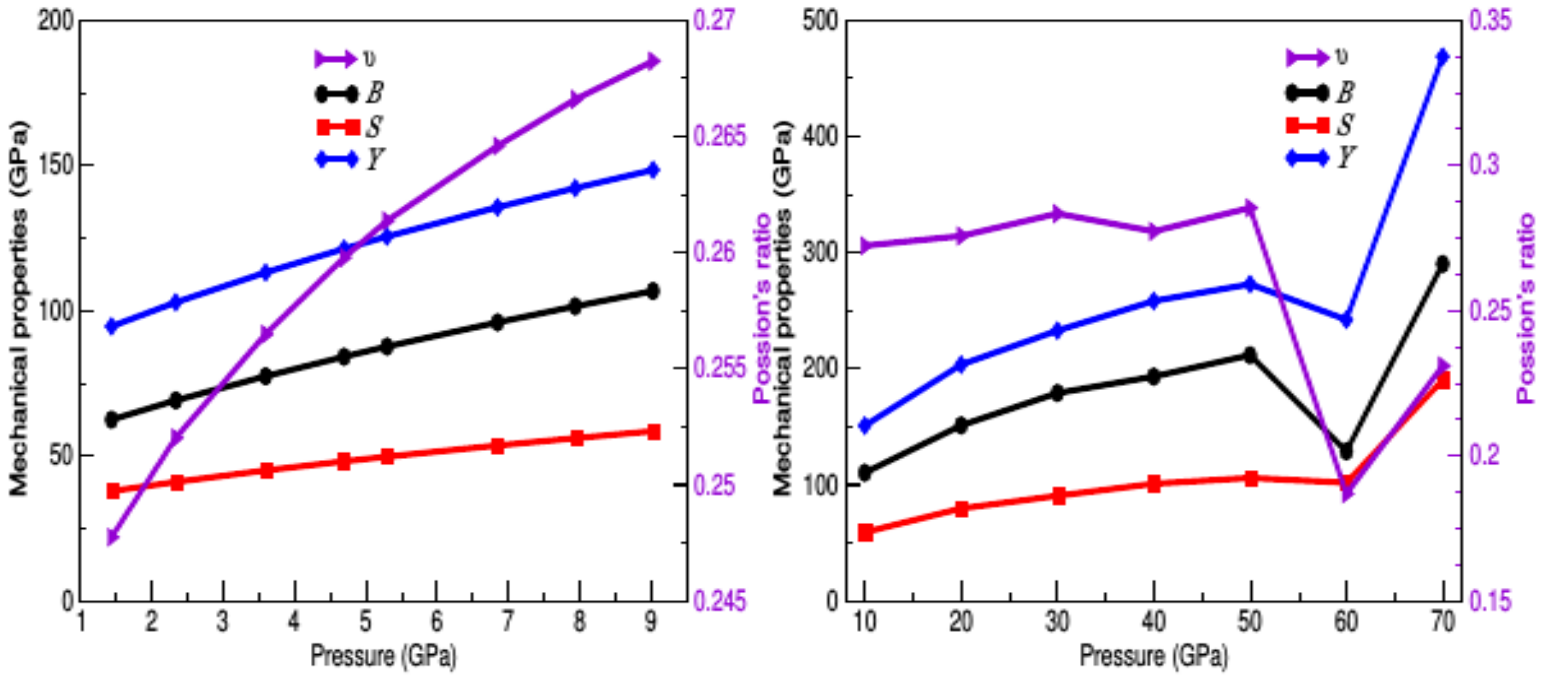
Electronic properties



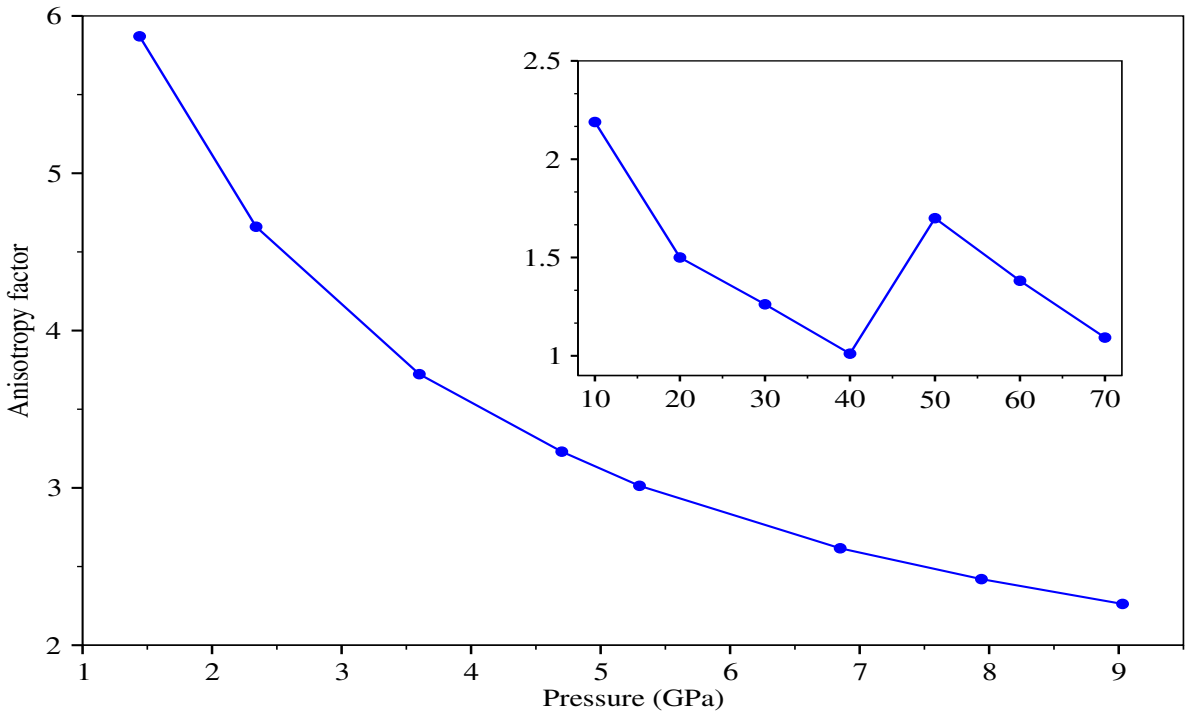
Mechanical stability: Mechanical stability



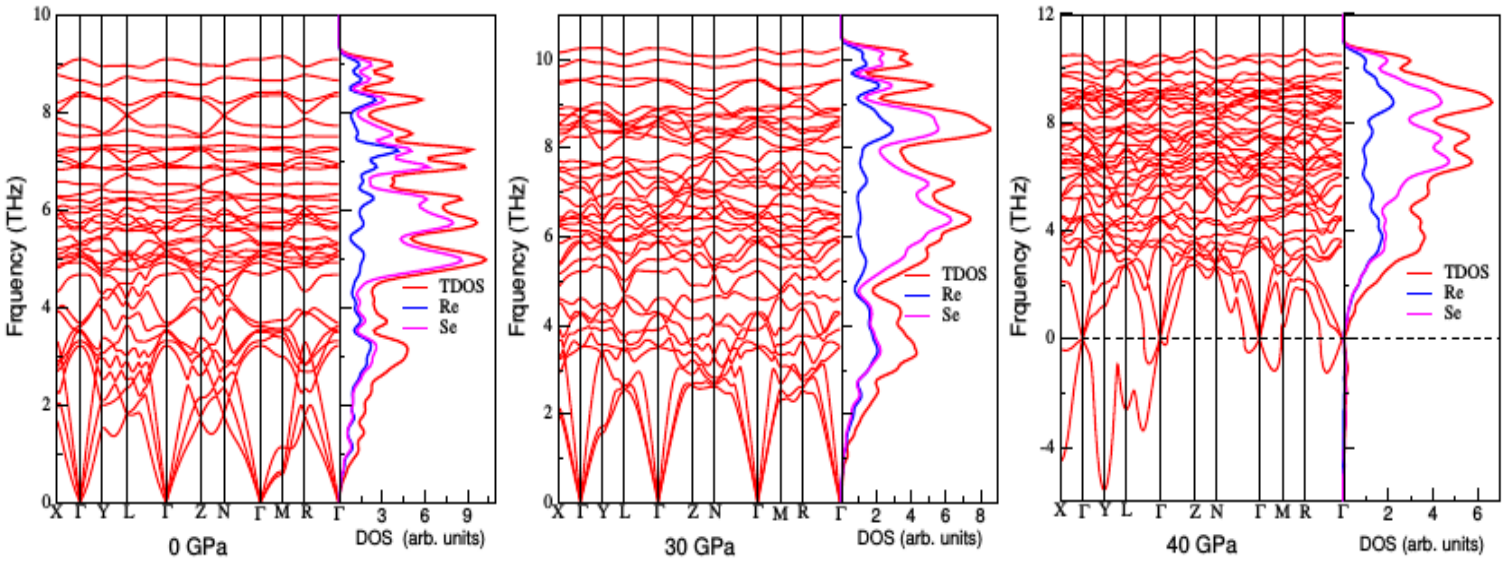
Mechanical stability: Mechanical stability



Mechanical stability: Zener anisotropy factor



Dynamical stability:



Conclusion

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We have investigated the structural, electronical, mechanical, and dynamical properties under pressure effect of bulk $ReSe_2$ from first principles. It is found that vdW force plays an important role in the inter-layer interaction of $ReSe_2$.

Thank You!

Acknowledgment