Pressure induced opto-electronic, elasto-mechanical and thermoelectric properties of cubic $FrBCl_3$ (B = Ge, Sn): DFT investigation

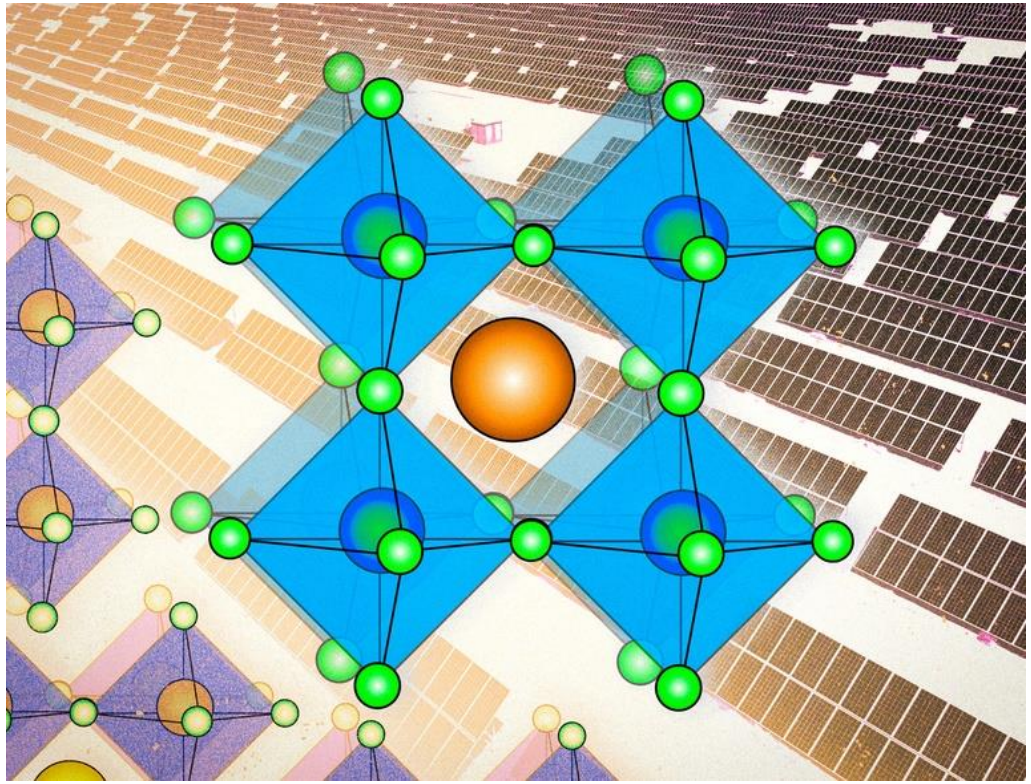
Mohammad Abdur Rashid

Md. Borhanul Asfia, Sahadat Jaman

Outline

- Lead-free perovskite
- Our systems of study: $FrGeCl_3$ and $FrSnCl_3$
- Computational details
- Opto-electronic properties
- Mechanical properties
- Thermoelectric properties
- Conclusions

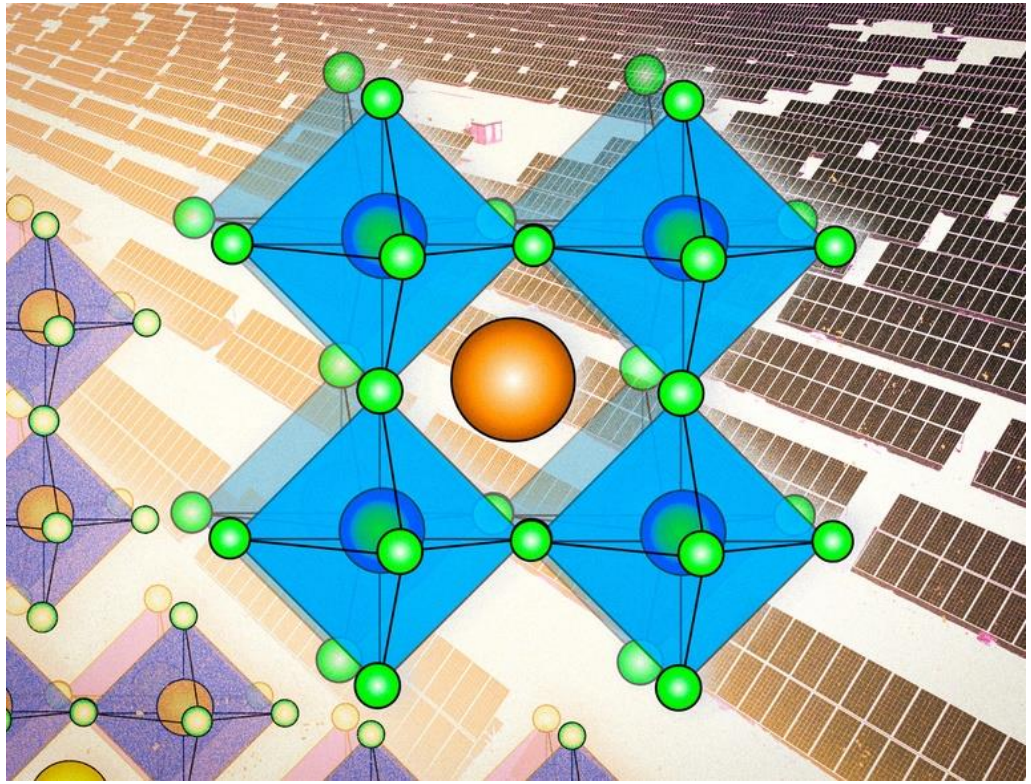
Perovskite solar cells



https://news.mit.edu/2022/perovskites-solar-cells-explained-0715

Perovskite solar cells

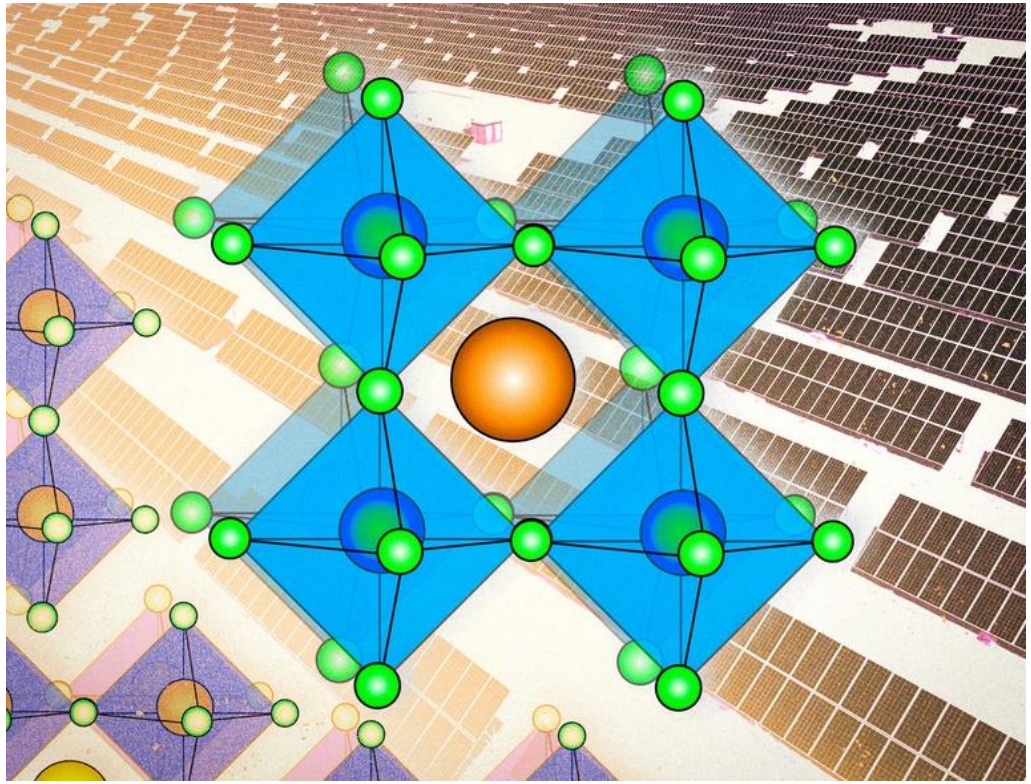
- High power conversion efficiency (about 25%)
- Easier manufacturing process
- Lower cost and greater flexibility



https://news.mit.edu/2022/perovskites-solar-cells-explained-0715

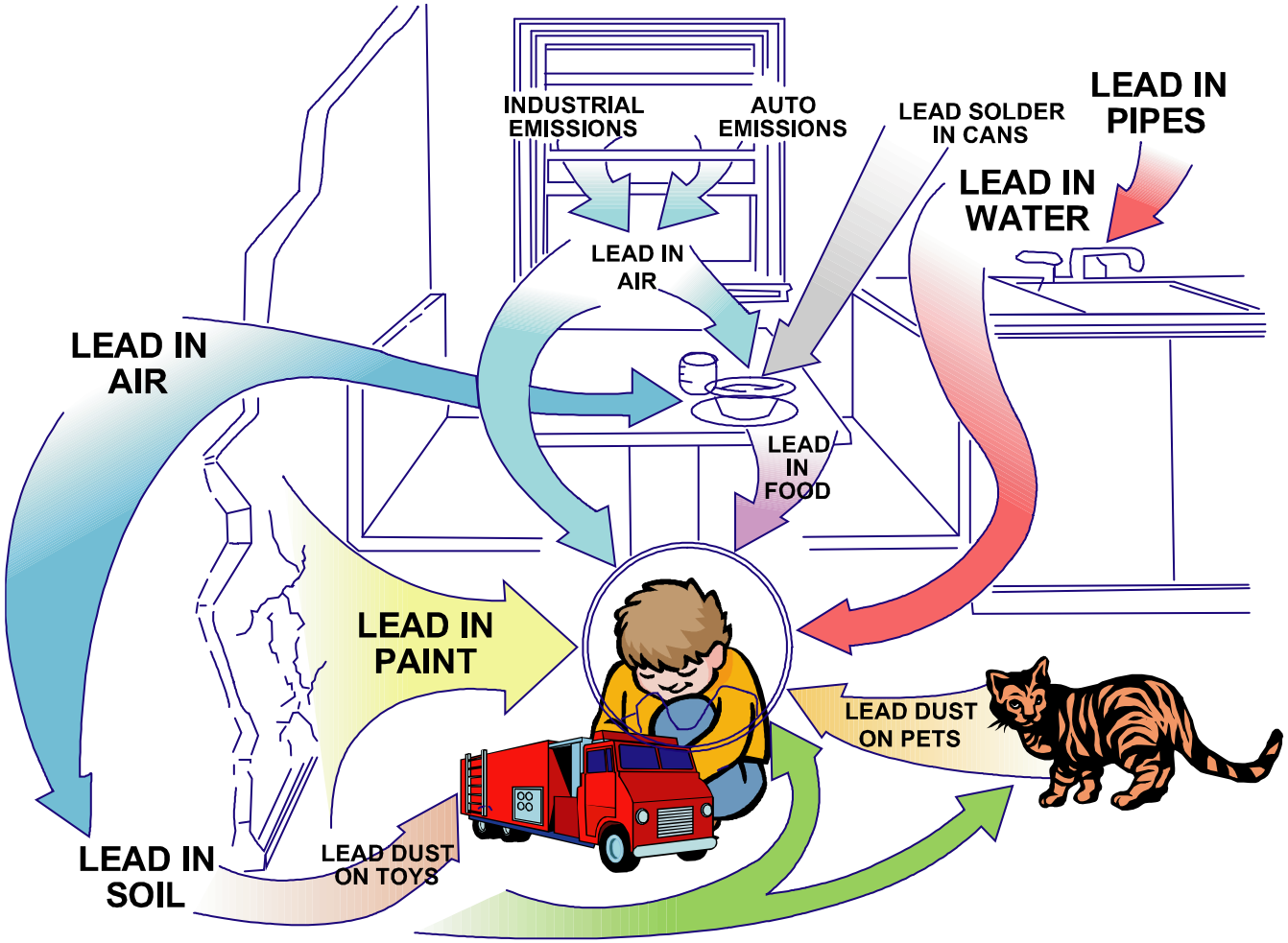
Perovskite solar cells

- High power conversion efficiency (about 25%)
- Easier manufacturing process
- Lower cost and greater flexibility
- Perovskites degrade much faster
- Pb-based perovskites show better potential but they are toxic



https://news.mit.edu/2022/perovskites-solar-cells-explained-0715

Environmental sources of lead exposure



https://www.cdc.gov/nceh/lead/publications/refugeetoolkit/powerpoint_files/medicalservice.ppt

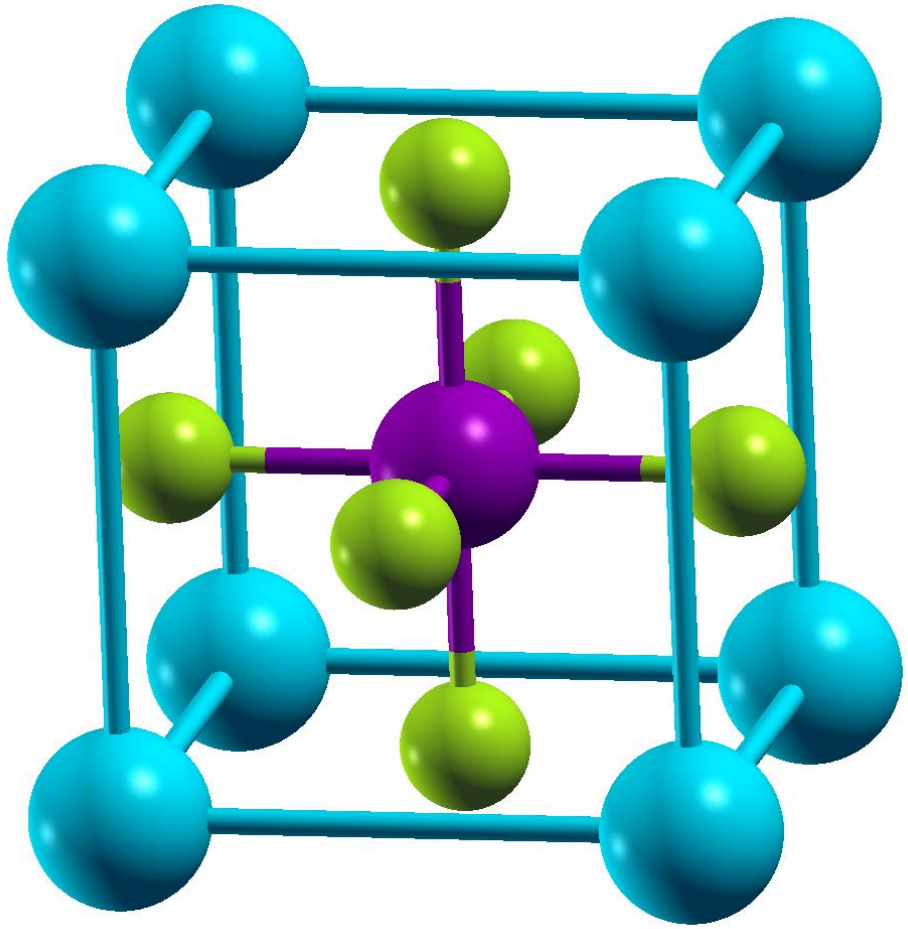
Structural, elastic and optoelectronic properties of inorganic cubic $FrBX_3$ (B = Ge, Sn; X = Cl, Br, I) perovskite: the density functional theory approach

Nazmul Hasan, [a] Md Arifuzzaman*[b] and Alamgir Kabir *[c]

Samples	Electronic bandgap, E_g (eV)
$FrGeCl_3$	1.14 eV
$FrGeBr_3$	0.81 eV
$FrGeI_3$	0.64 eV
$FrSnCl_3$	1.05 eV
$FrSnBr_3$	0.67 eV
$FrSnI_3$	0.42 eV

RSC Advances, 2022, 12, 7961

Structure of $FrBCl_3$ (B = Ge, Sn)

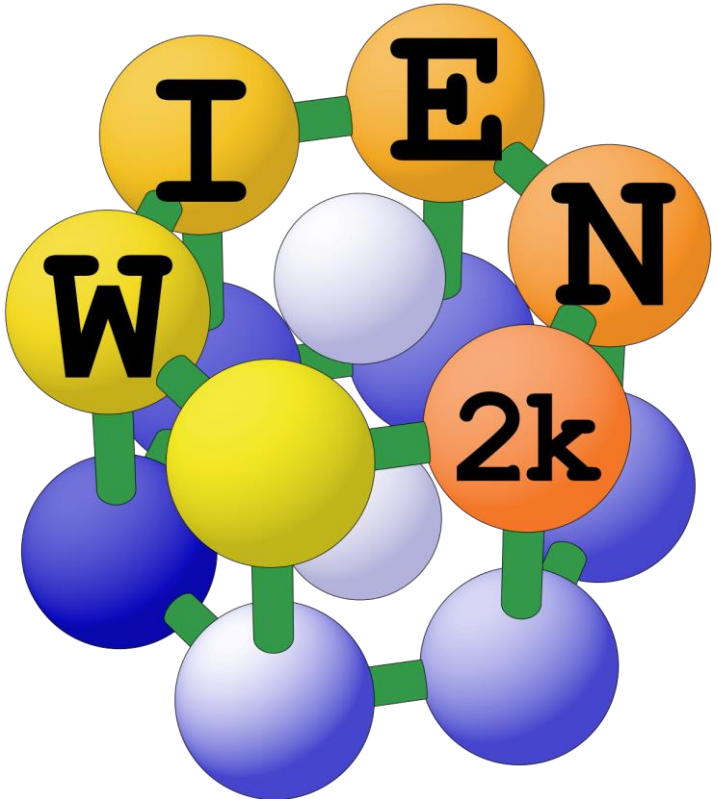


Fr

Ge/Sn

Cl

Computational details

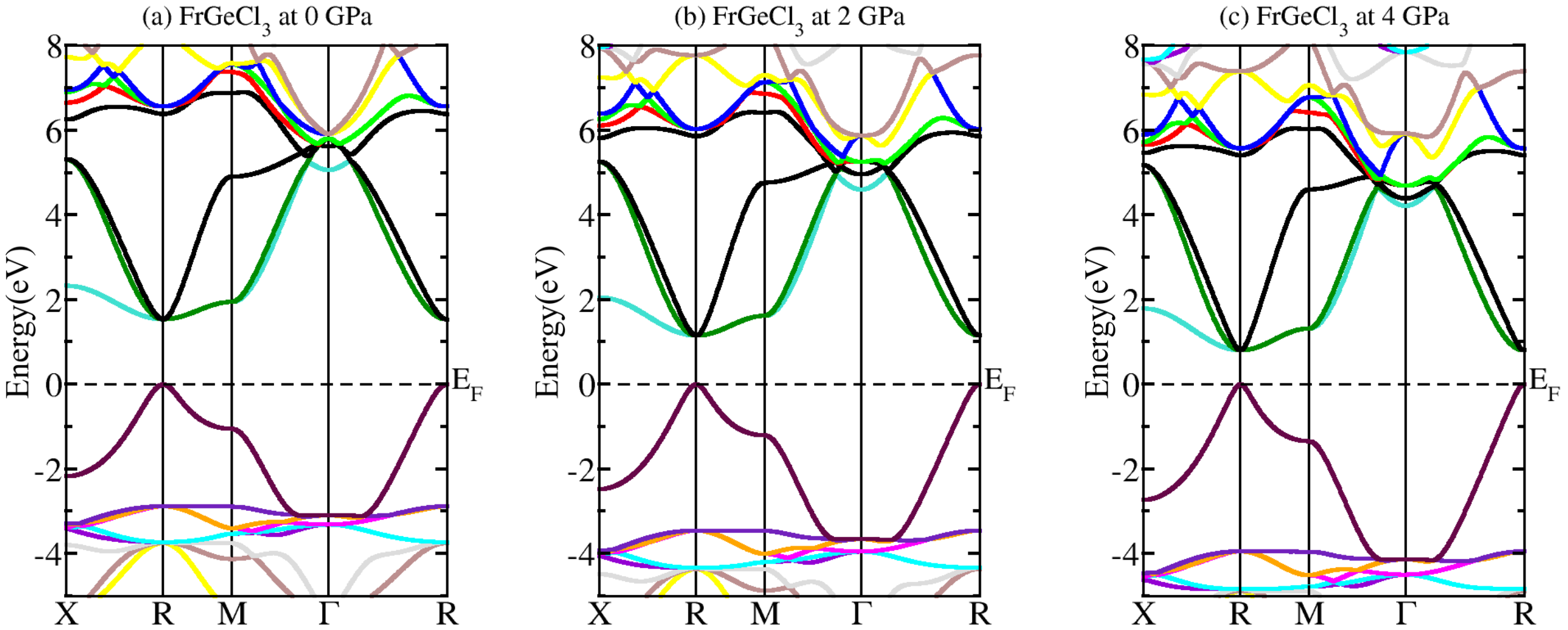


- R_{MT}(Fr, Sn, Ge) = 2.35 a.u.
- R_{MT} (Cl) = 2.32 a.u.
- $R_{MT} \times K_{max}$ = 8.0
- K-mesh = 10×10×10
- EC = 0.00001 Ry & CC = 0.0001 *e*

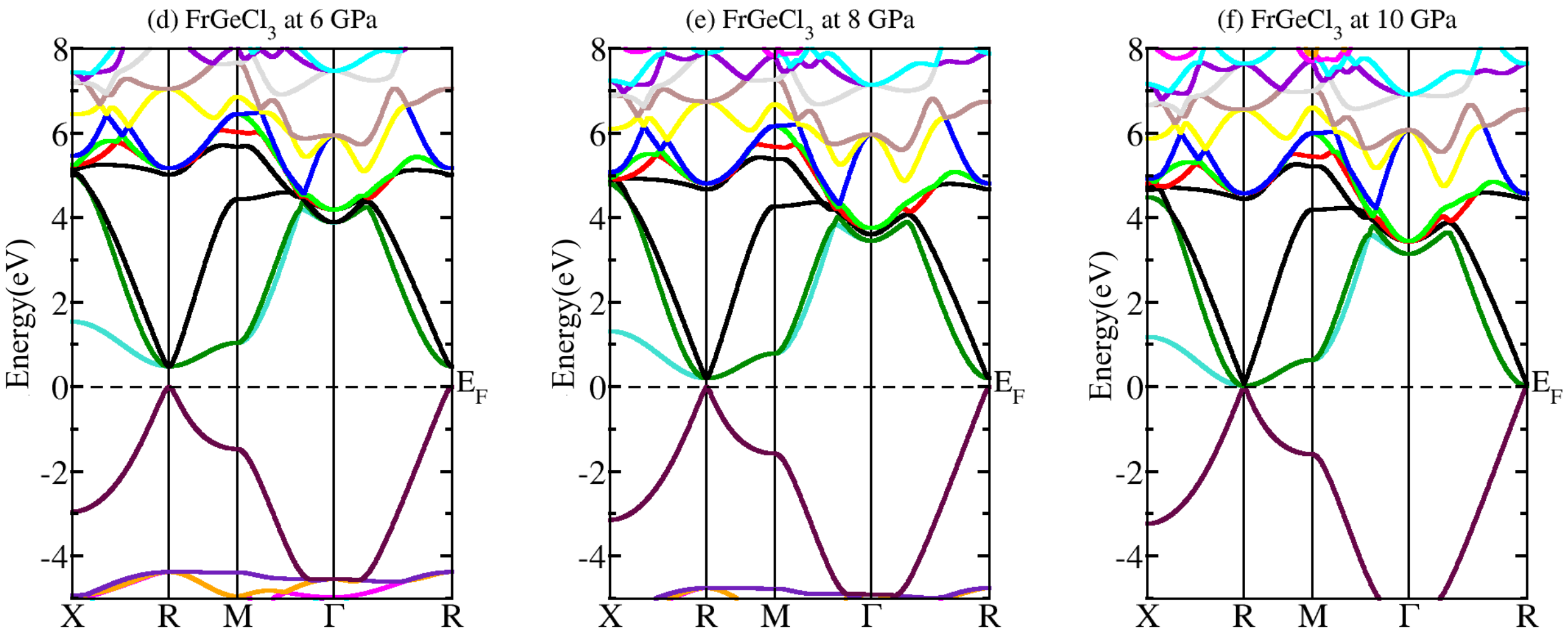
Optimized Lattice parameters and estimated E_g

Pressure (GPa)	Lattice Parameter (Å)		Bandgap (eV) with mBJ potential	
	$FrGeCl_3$	$FrSnCl_3$	$FrGeCl_3$	$FrSnCl_3$
0	5.375	5.648	1.540	1.546
2	5.259	5.499	1.154	1.047
4	5.169	5.373	0.807	0.547
6	5.096	5.265	0.494	0.054
8	5.034	5.171	0.207	0.000
10	4.981	-	0.000	-

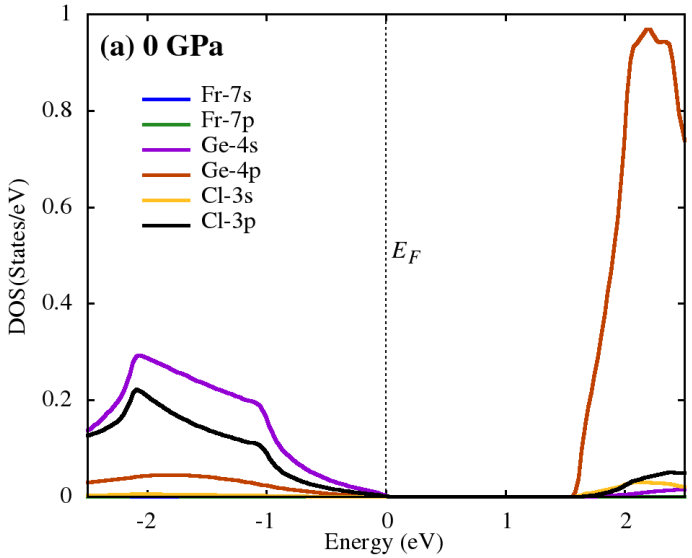
Electronic properties of $FrGeCl_3$

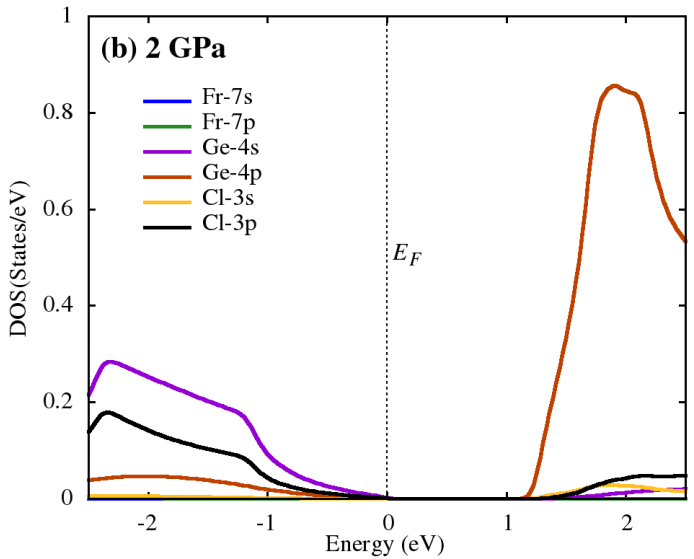


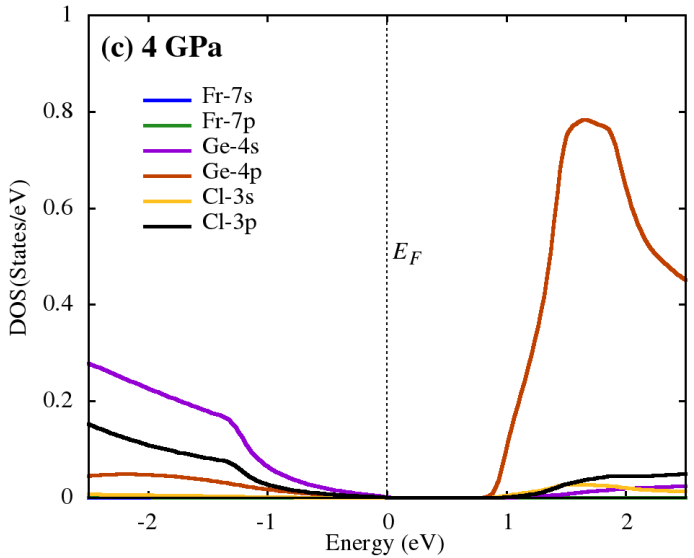
Electronic properties of $FrGeCl_3$

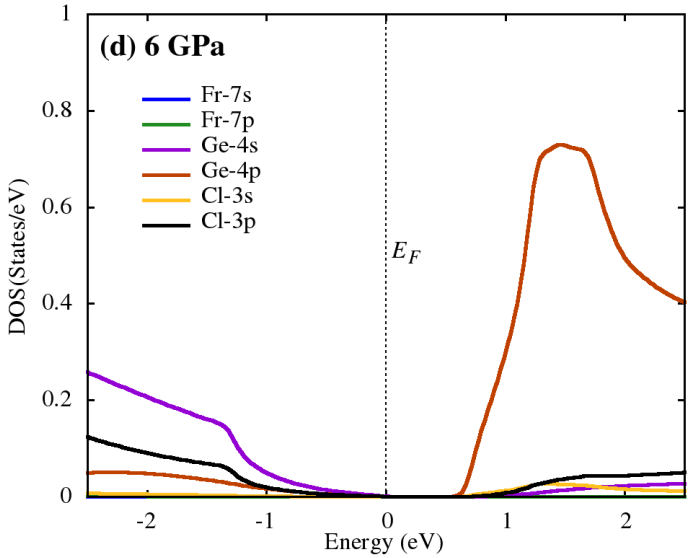


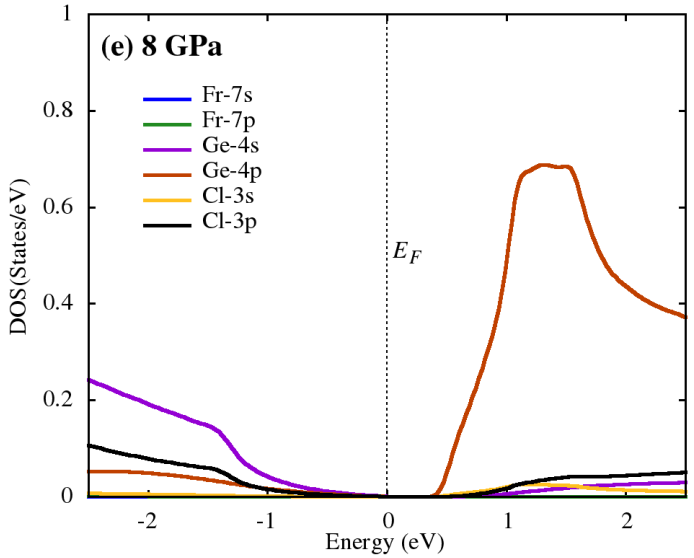
Electronic properties of $FrGeCl_3$

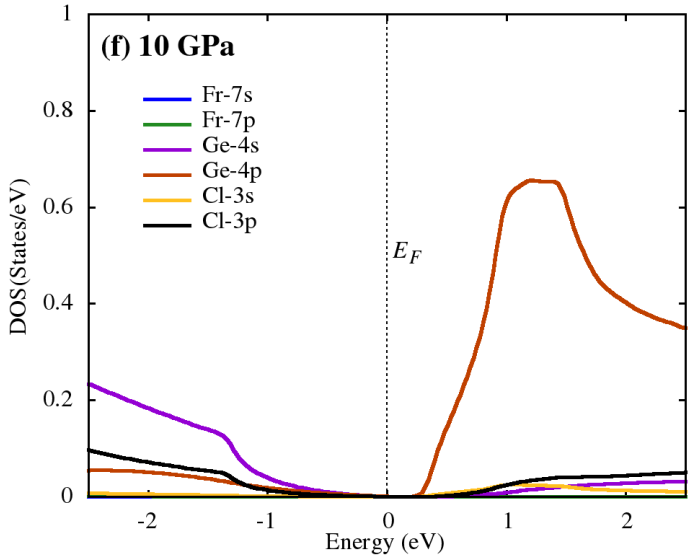




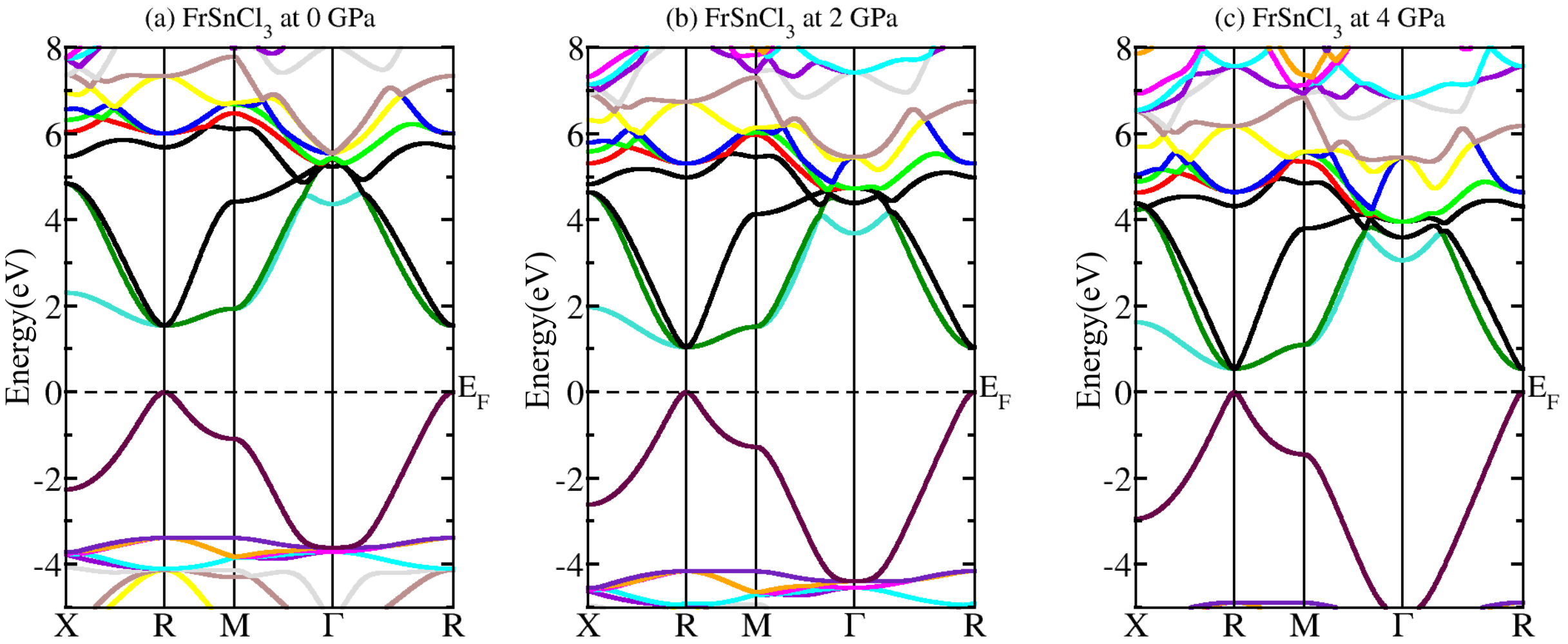




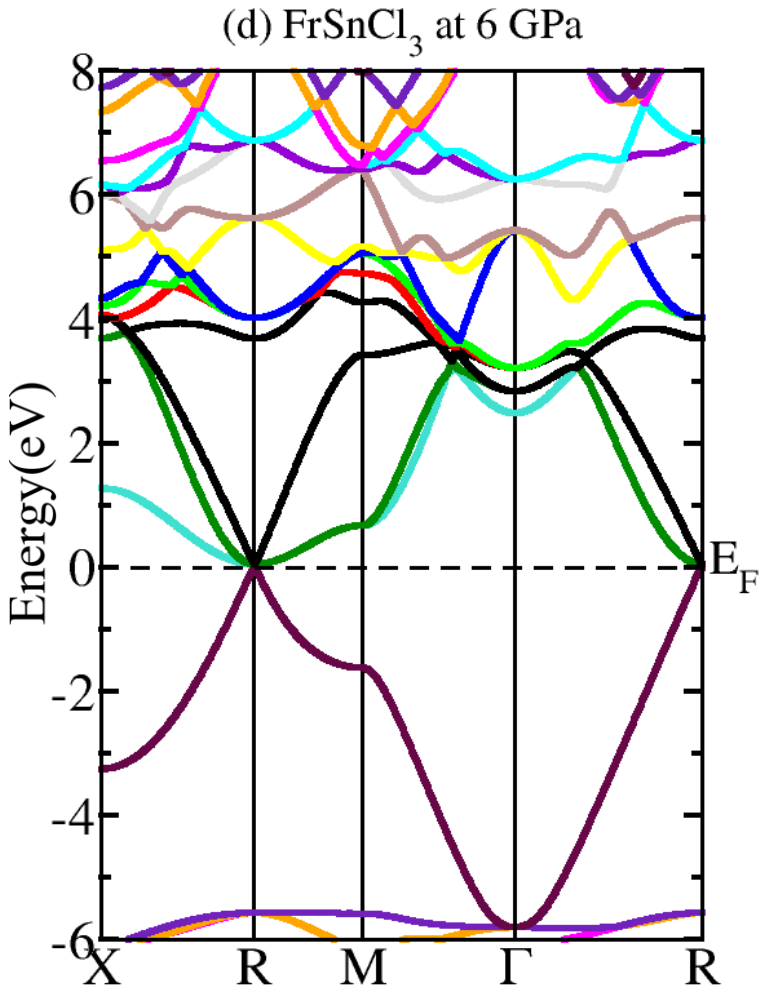


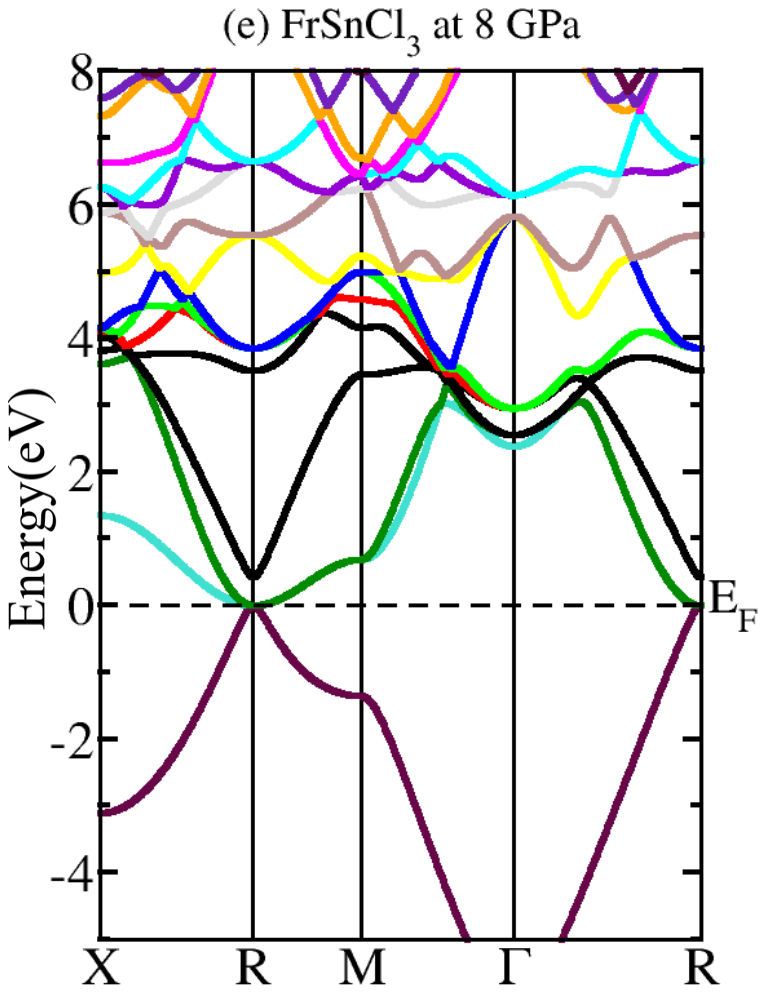


Electronic properties of $FrSnCl_3$

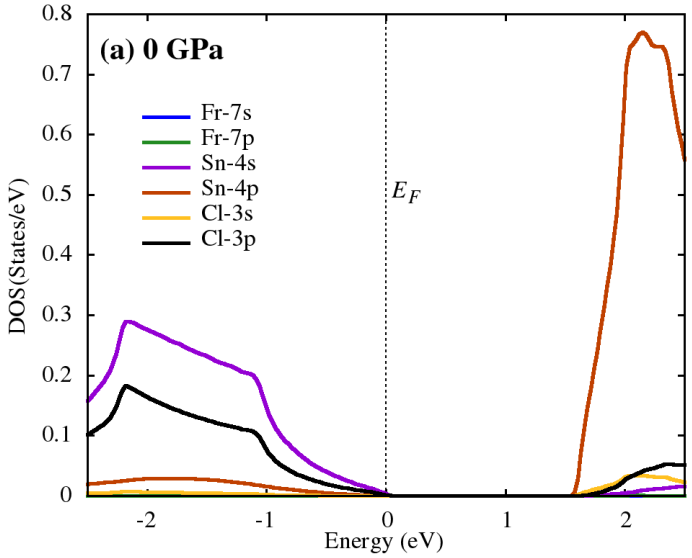


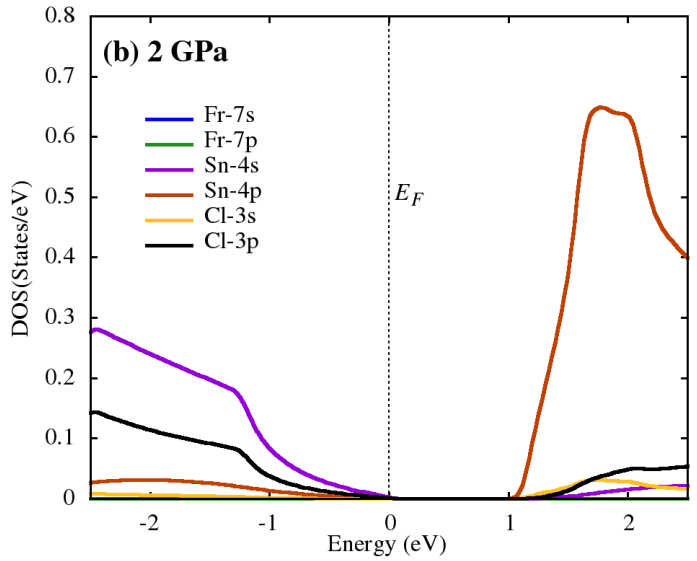
Electronic properties of $FrSnCl_3$

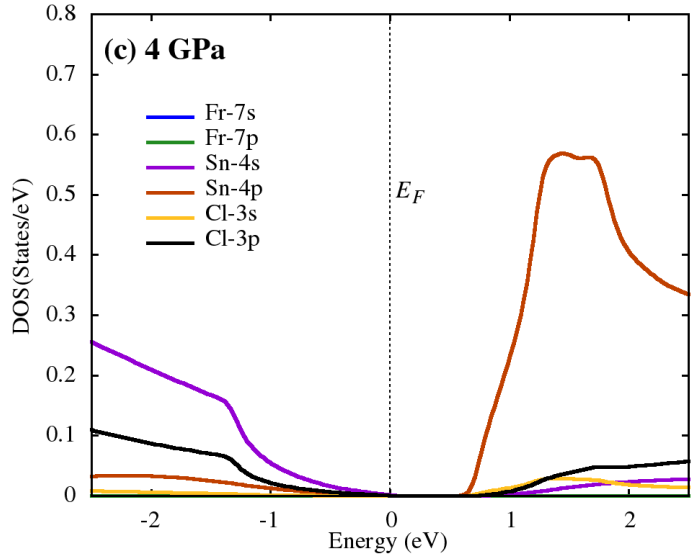


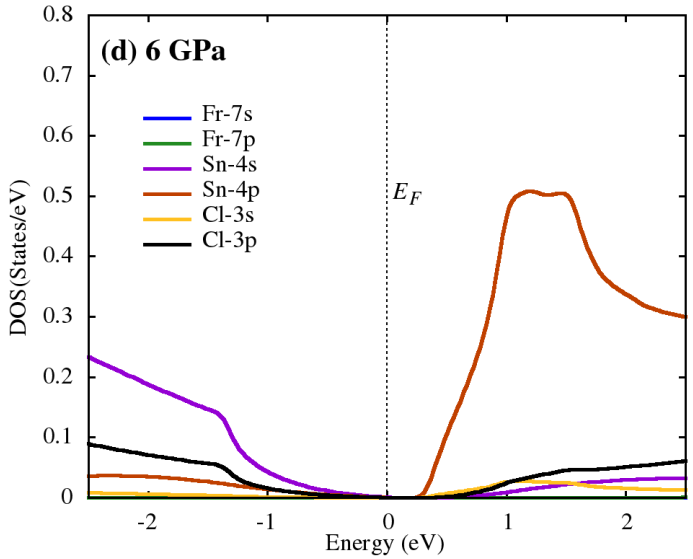


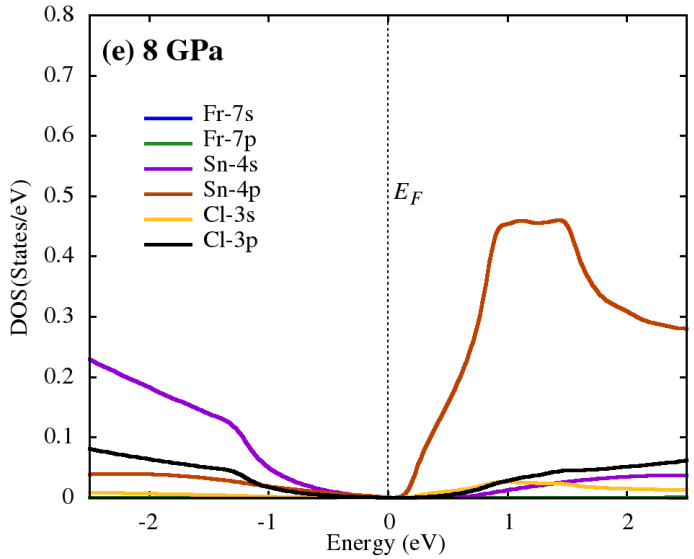
Electronic properties of $FrSnCl_3$



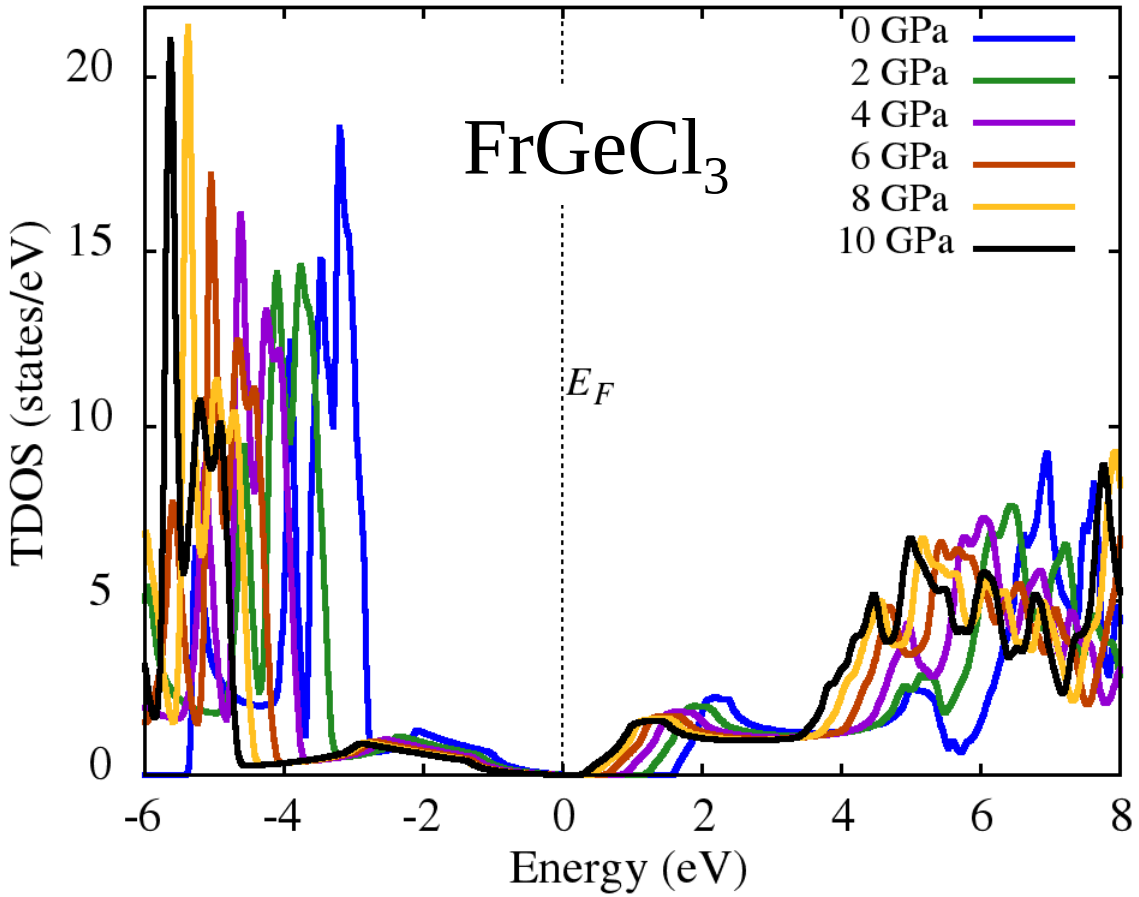


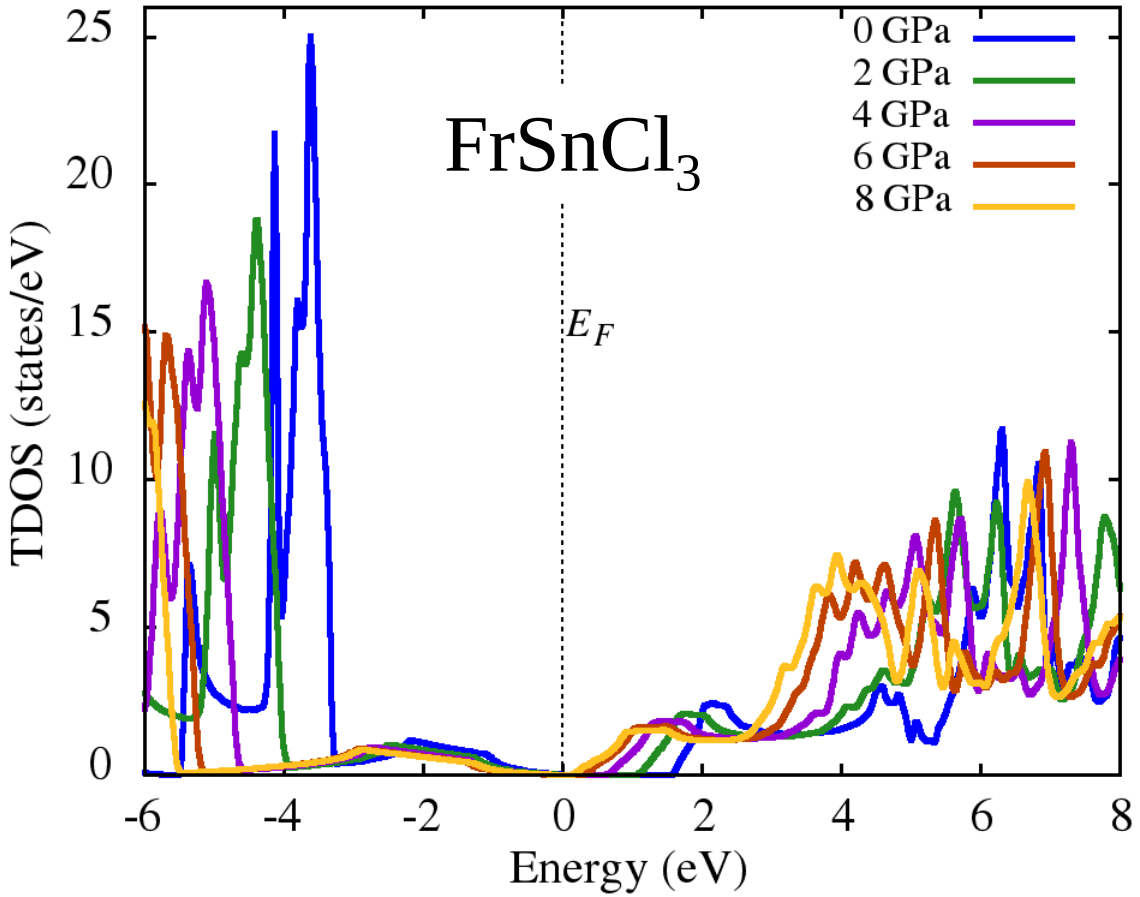






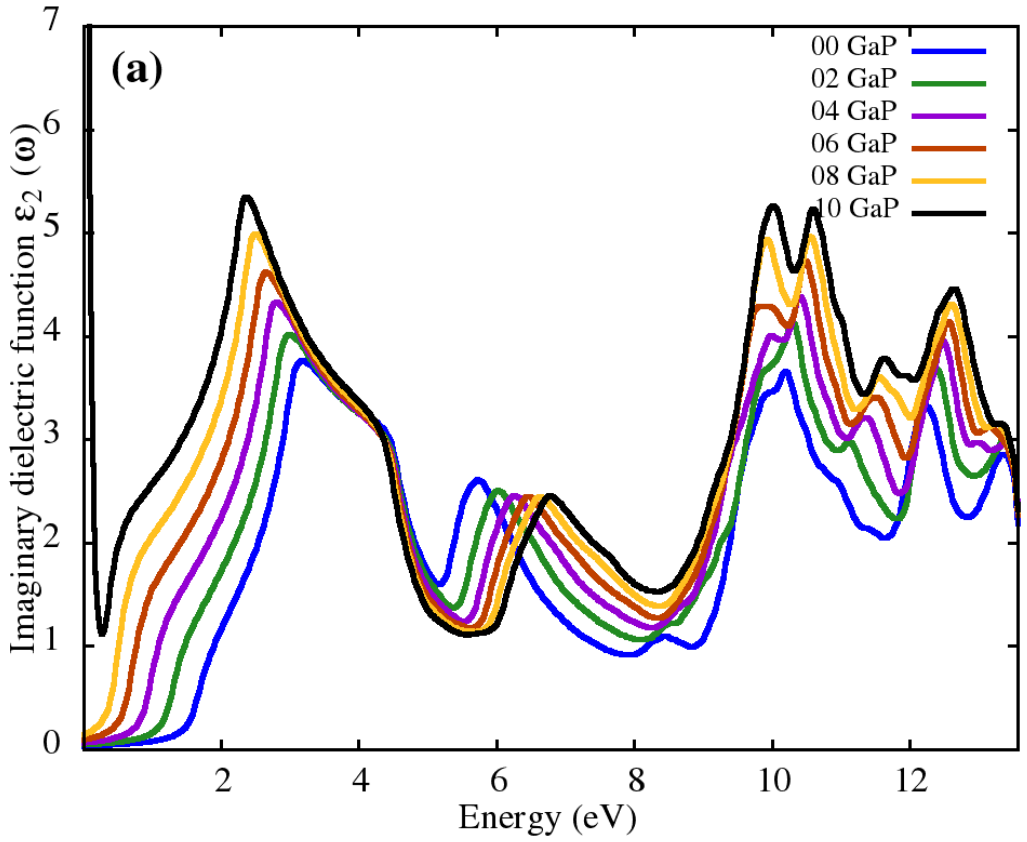
Electronic properties

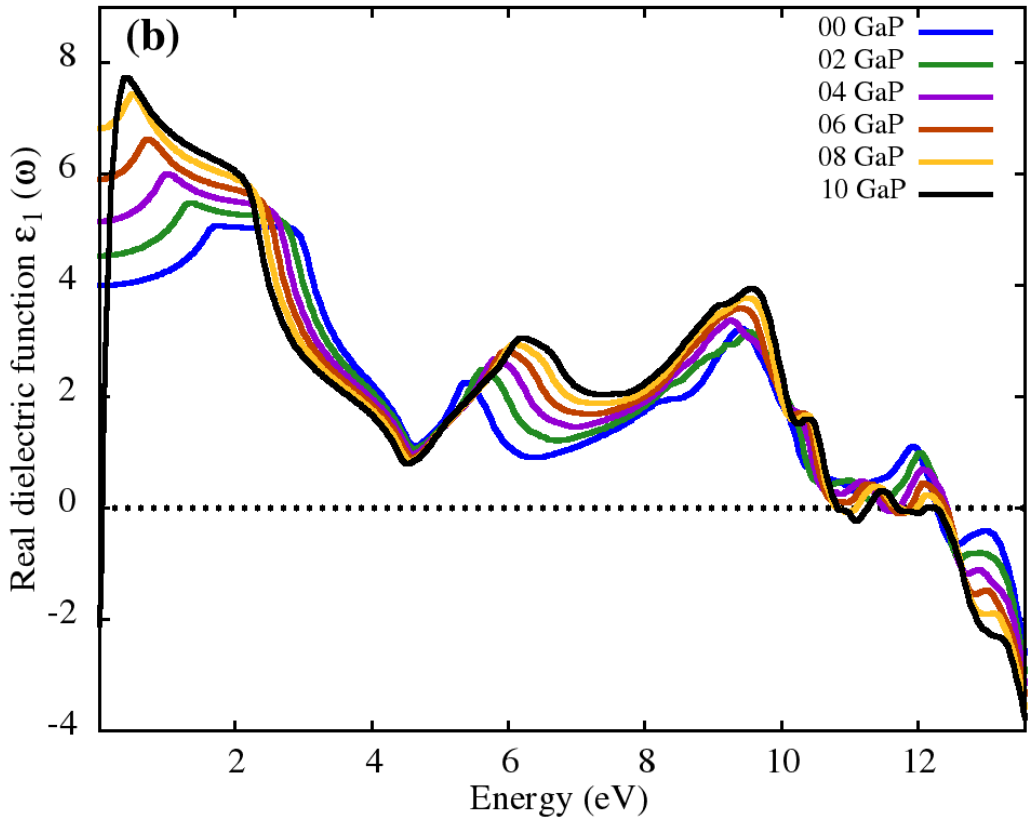




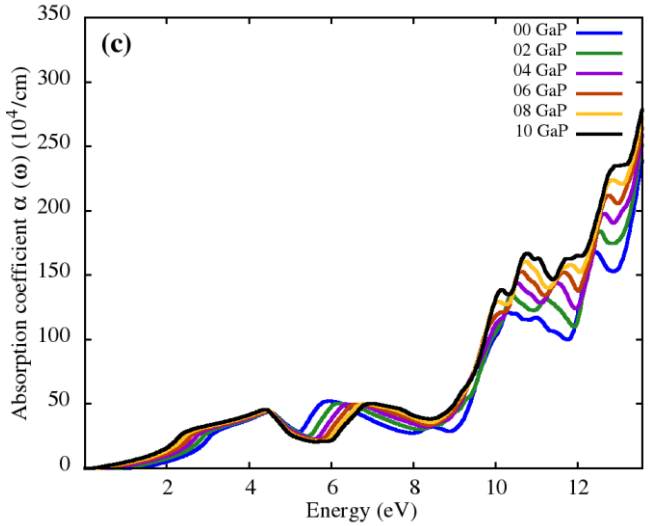
Optical properties of $FrGeCl_3$

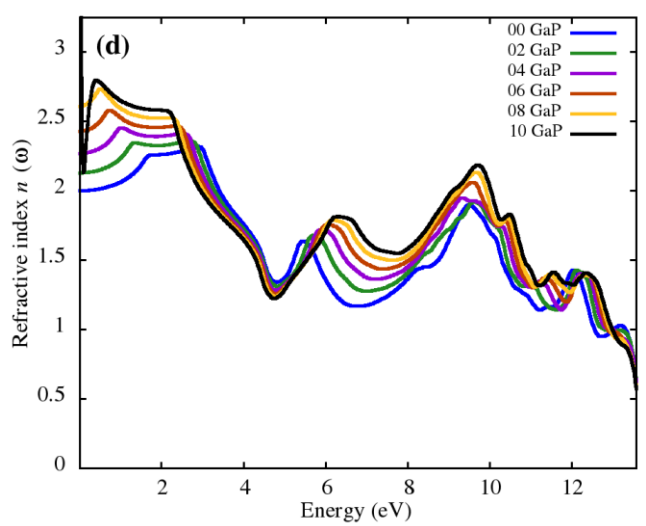
$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

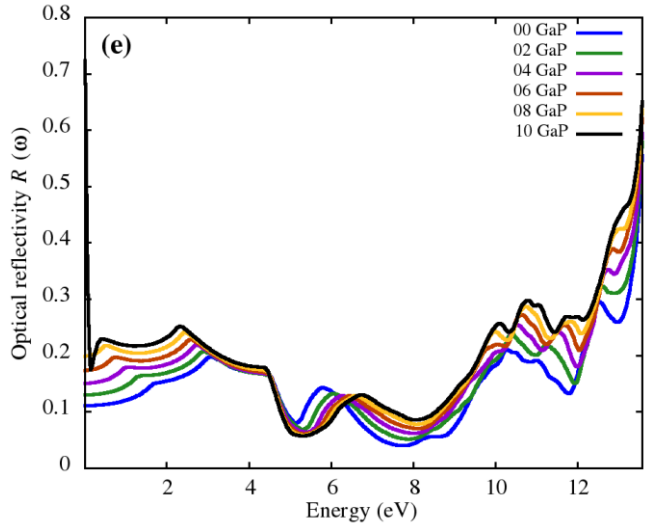


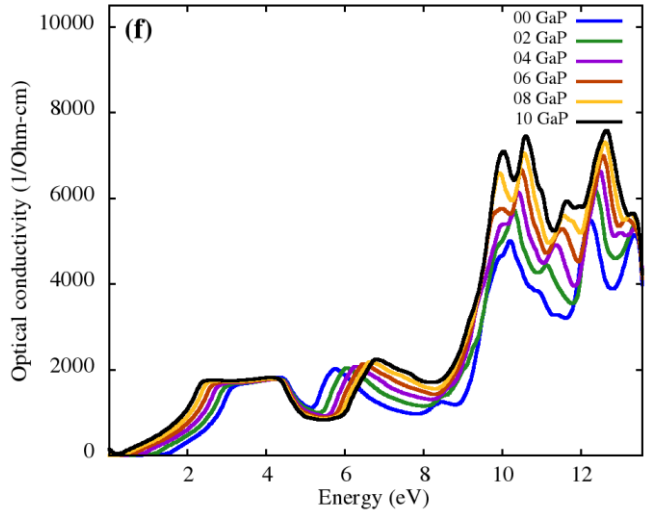


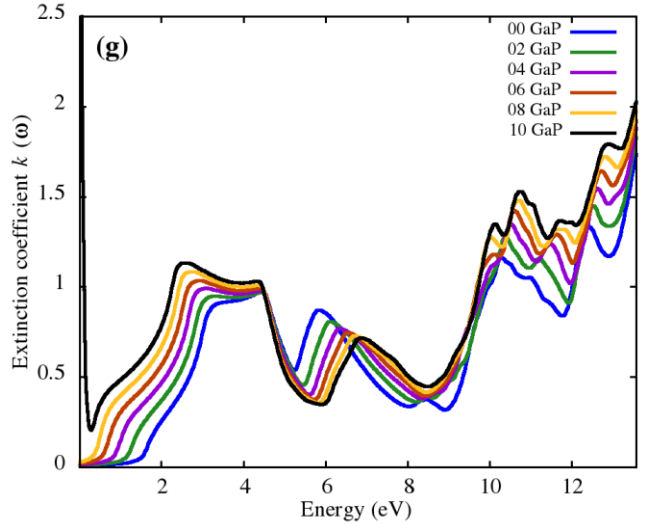
Optical properties of $FrGeCl_3$

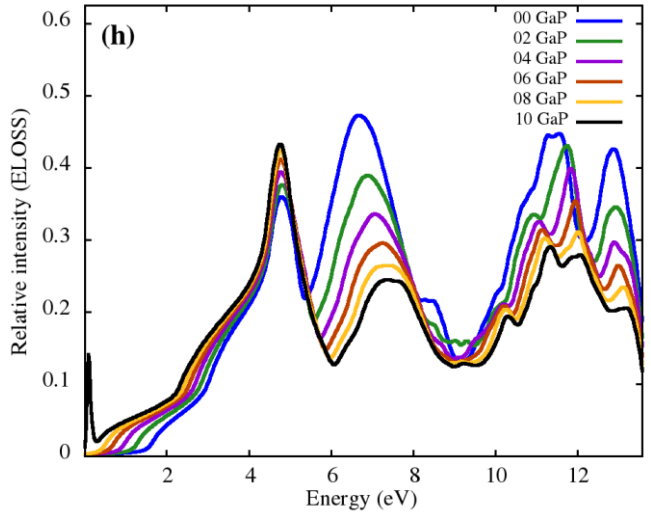






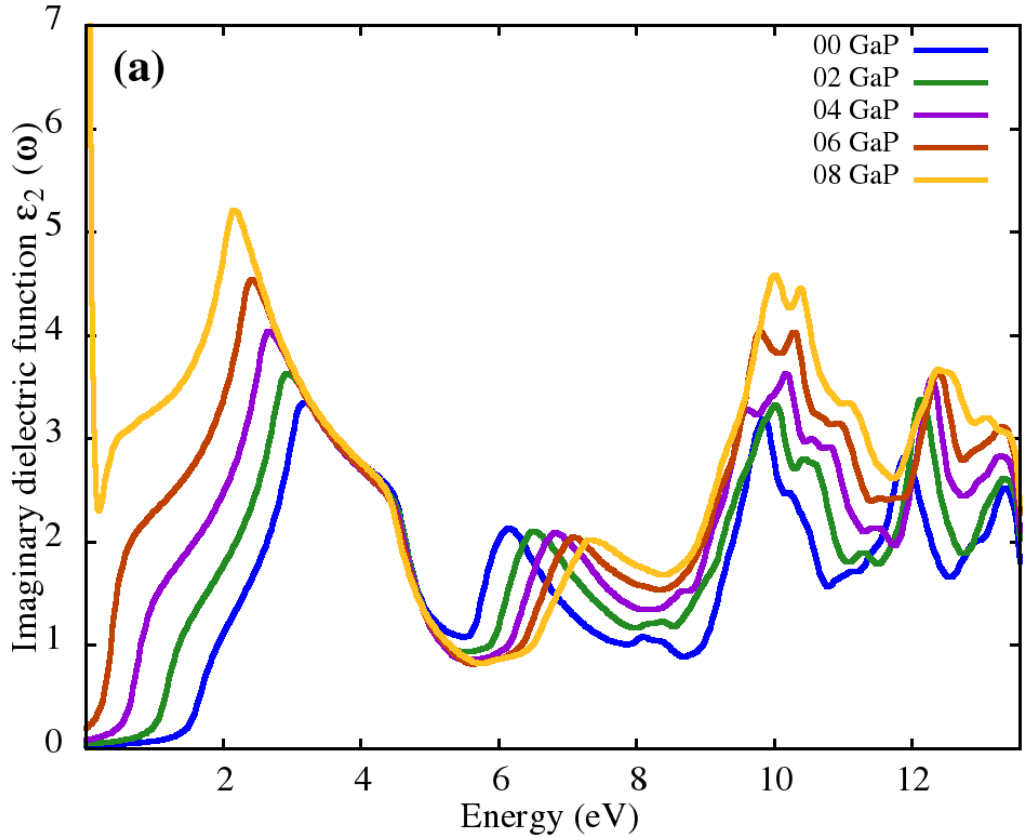


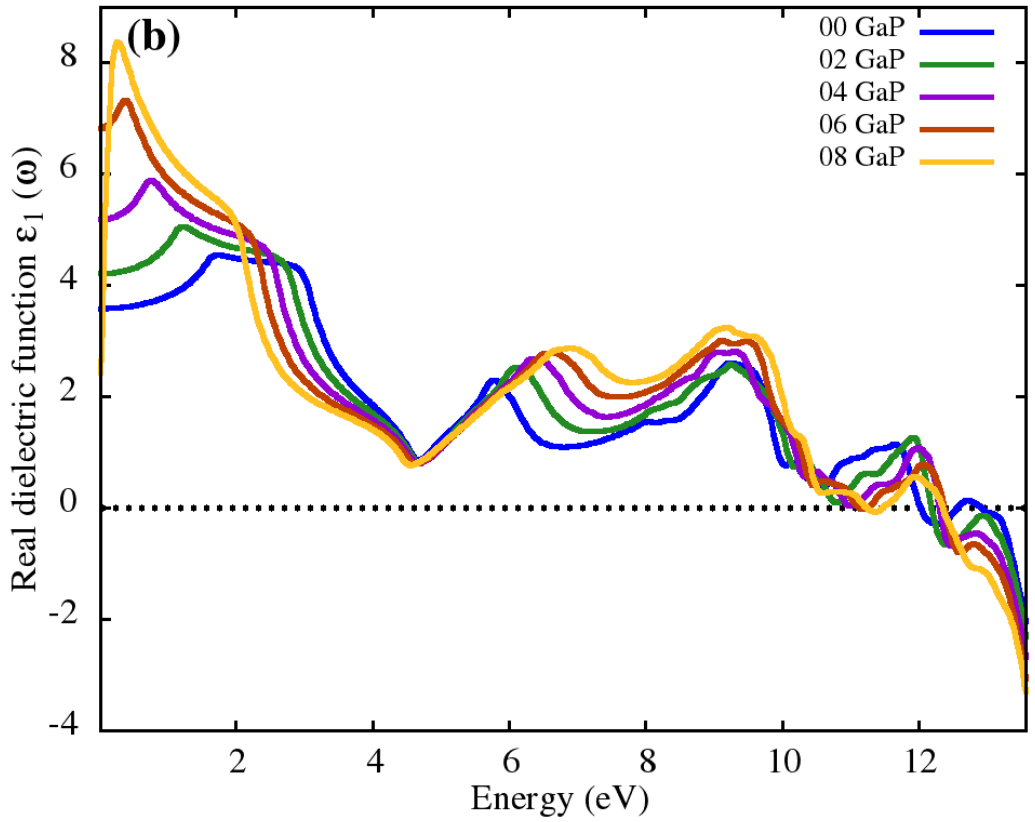




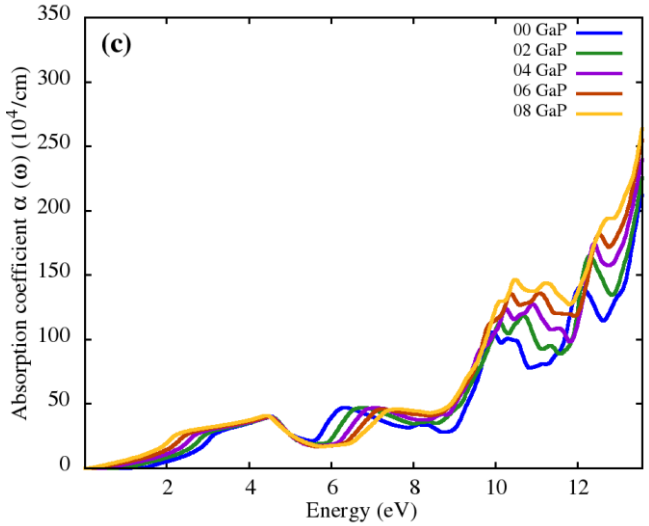
Optical properties of $FrSnCl_3$

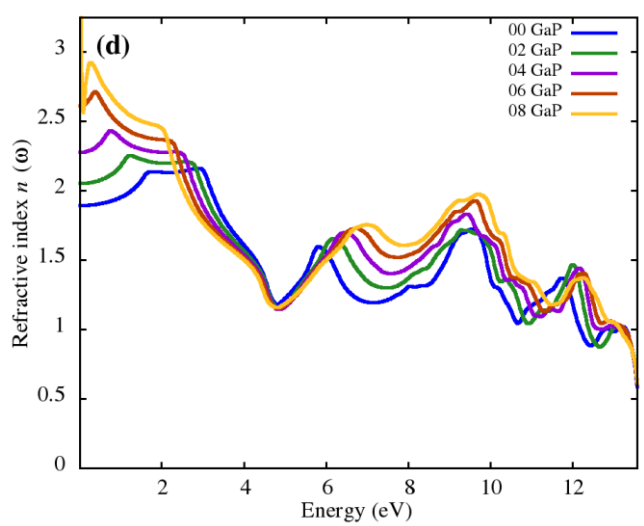
$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

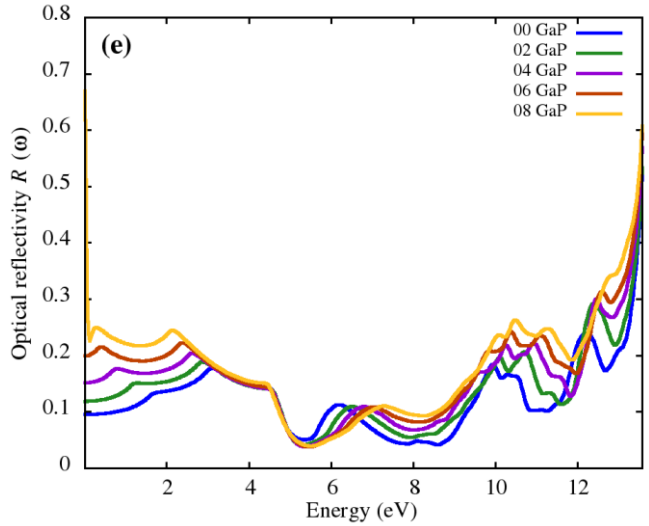


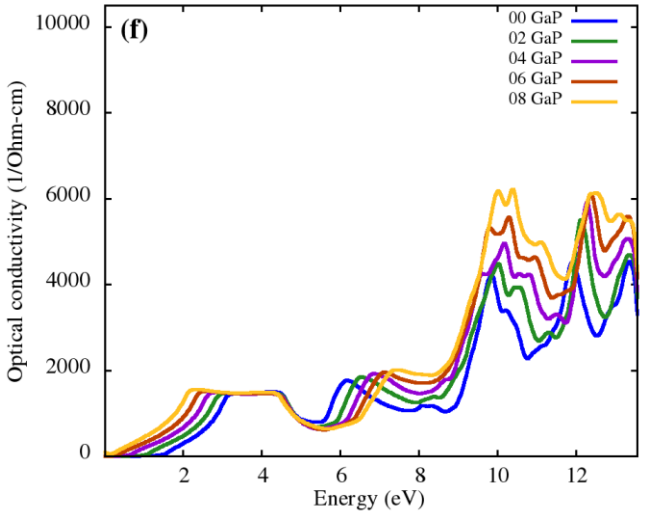


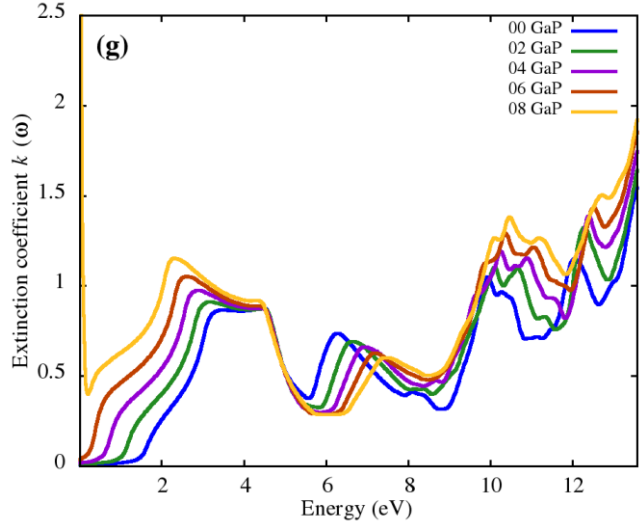
Optical properties of $FrSnCl_3$

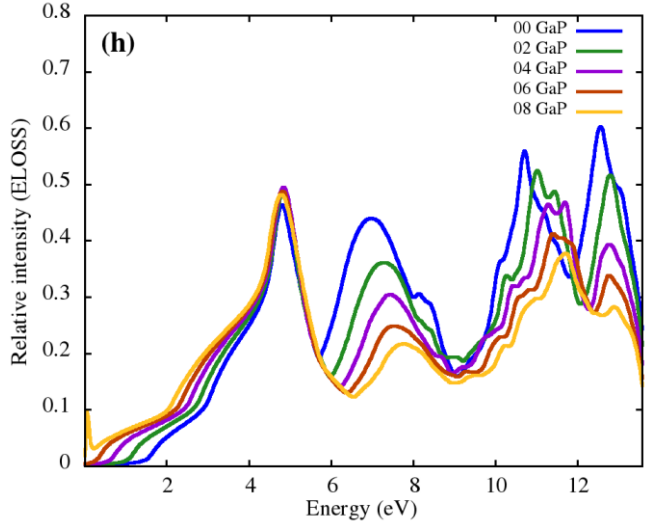








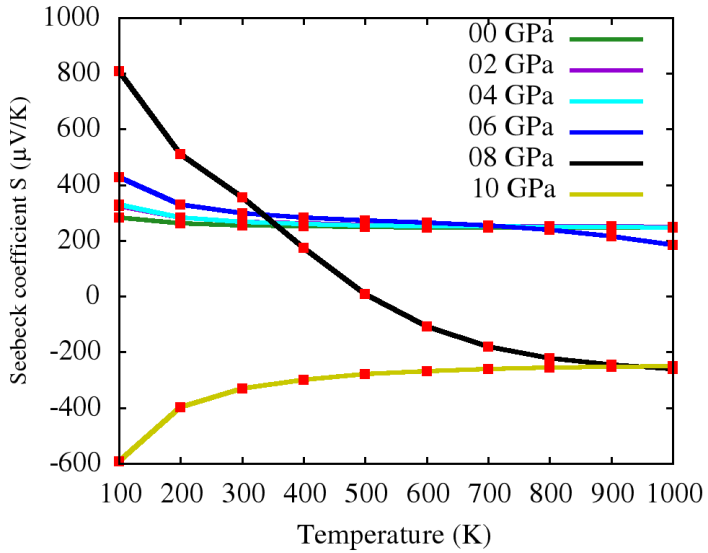


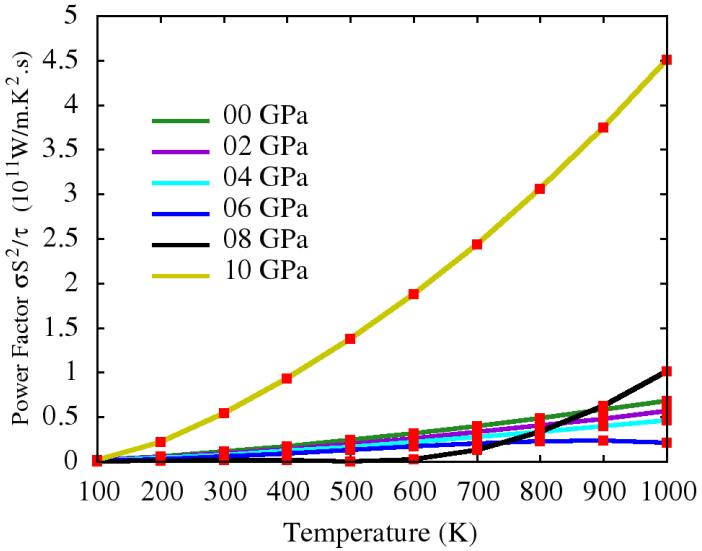


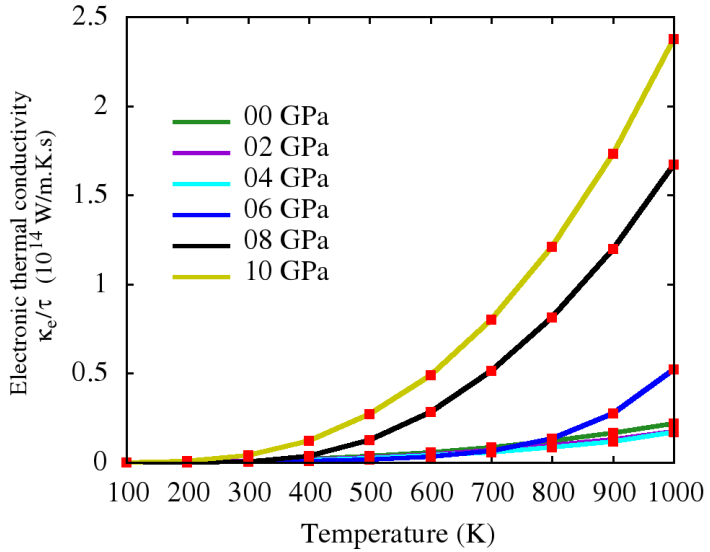
Mechanical properties of $FrBCl_3$ (B = Ge, Sn)

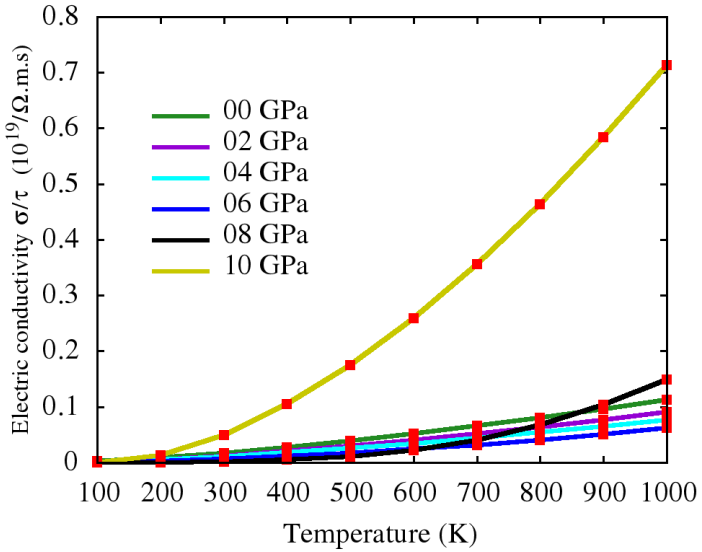
System	Pressure (GPa)	C_{11}	C_{12}	C_{44}	B (GPa)	G (GPa)	Y (GPa)	B/G	v
$FrGeCl_3$	0	51.86	13.01	10.79	25.96	14.24	36.12	1.823	0.27
	2	68.73	17.08	12.07	34.30	17.57	45.03	1.952	0.28
	4	84.69	20.61	13.88	41.97	21.15	54.32	1.985	0.28
	6	102.41	22.86	15.69	49.38	25.32	64.88	1.950	0.28
	8	136.82	50.68	15.04	79.39	26.25	70.93	3.025	0.35
	10	125.02	29.01	15.34	61.01	28.41	73.77	2.148	0.30
$FrSnCl_3$	0	44.44	8.62	5.96	20.56	10.74	27.44	1.915	0.28
	2	73.35	12.14	10.11	32.54	18.31	46.25	1.777	0.26
	4	88.38	15.45	4.12	39.76	17.05	44.76	2.331	0.31
	6	108.25	18.22	4.81	48.23	20.89	54.76	2.309	0.31
	8	135.07	22.81	4.68	60.23	25.26	66.49	2.384	0.32

Thermoelectric properties of $FrGeCl_3$

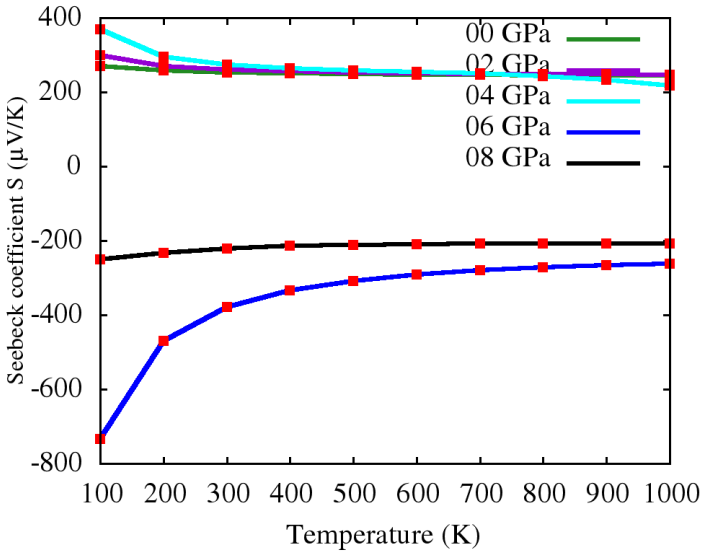


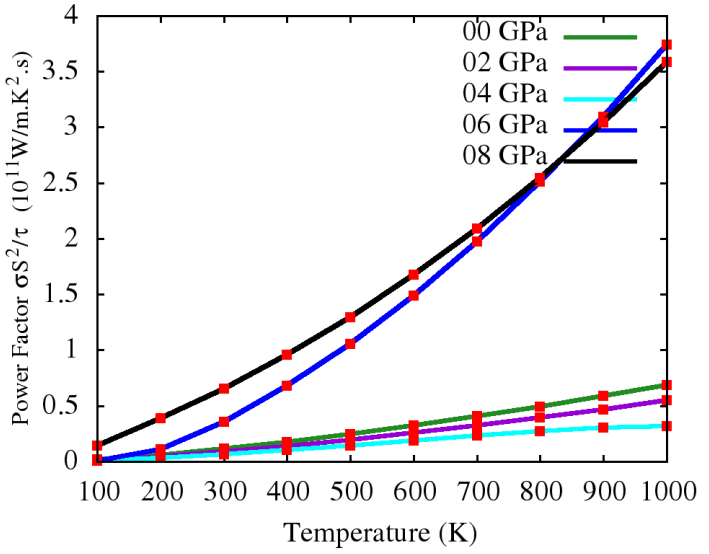


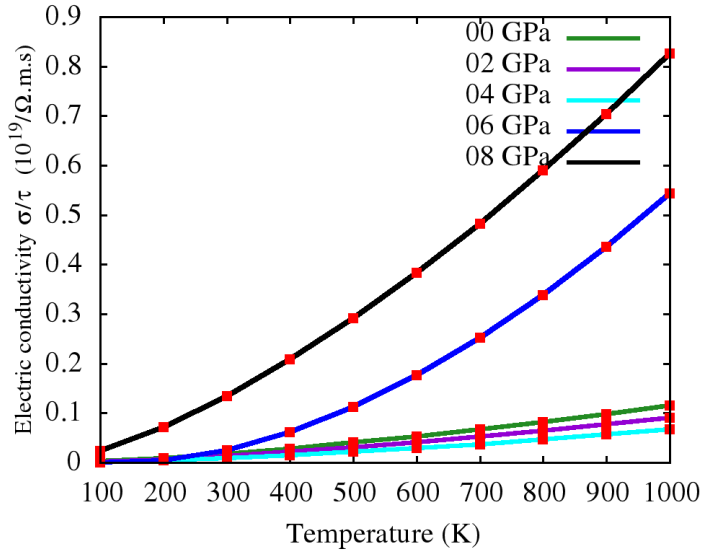


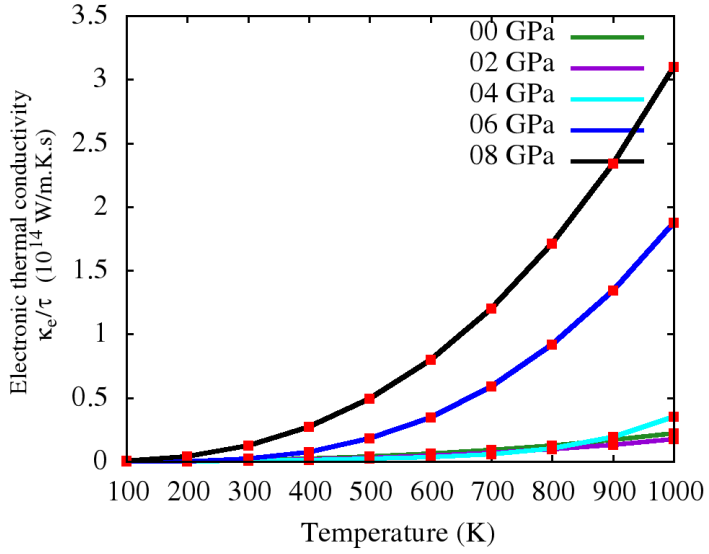


Thermoelectric properties of $FrSnCl_3$









Conclusions

- Opto-electronic and thermoelectric properties perovskites of $FrBCl_3$ (B = Ge, Sn) using WIEN2k
- Both compounds show semiconductor like behavior
- Remarkable optical properties and ductile in nature
- Good Seebeck coefficient and power factor
- Promising materials for different opto-electronic and thermoelectric applications


“Thank you”