

## **Pressure-Induced Multi-Functional Property Analysis of Lead Free Tin Based Halide Perovskites $\text{ASnCl}_3$ (A = Ga, In, Tl) for Advanced Optoelectronic Applications**

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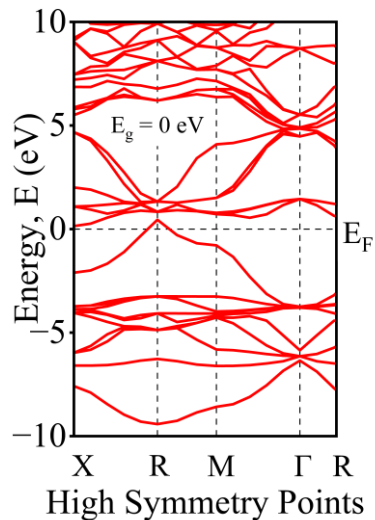
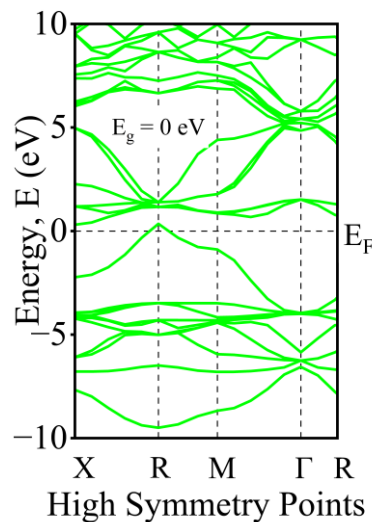
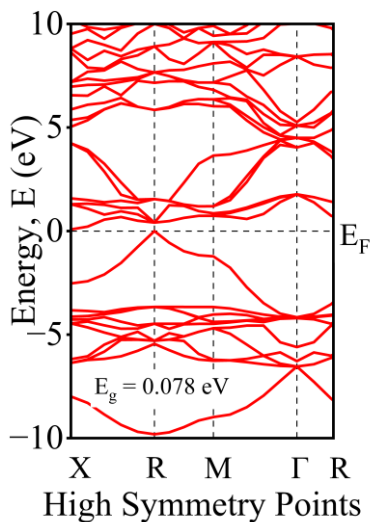
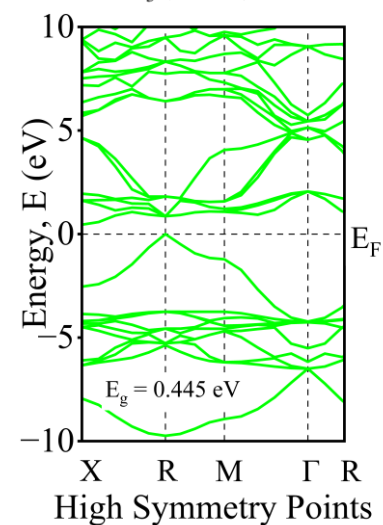
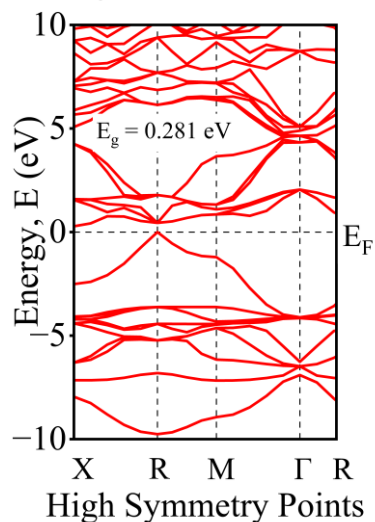
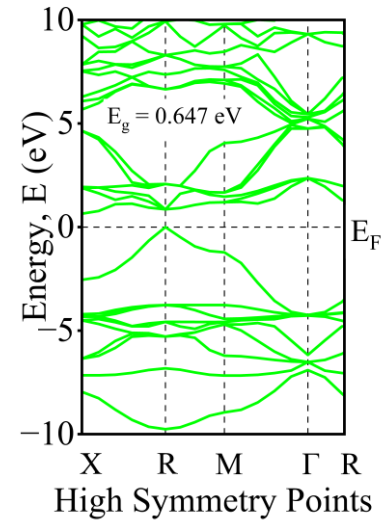
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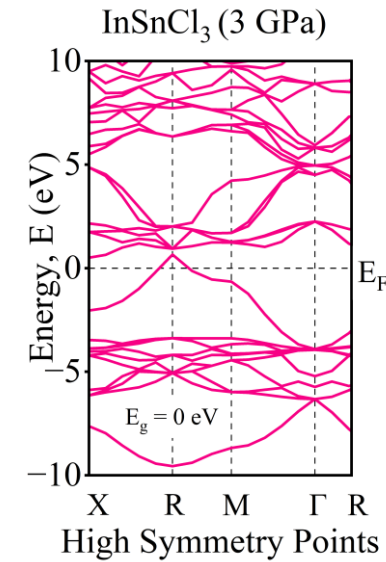
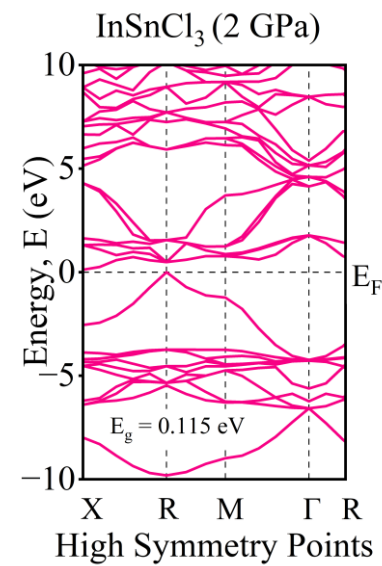
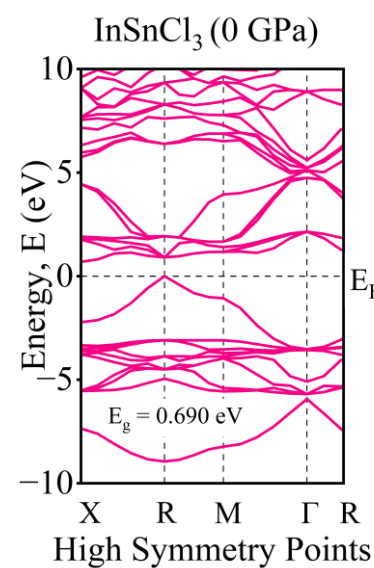
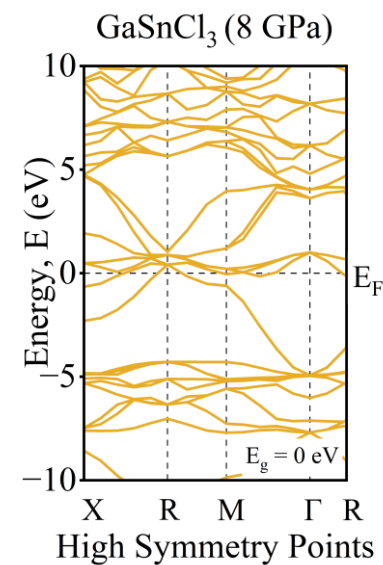
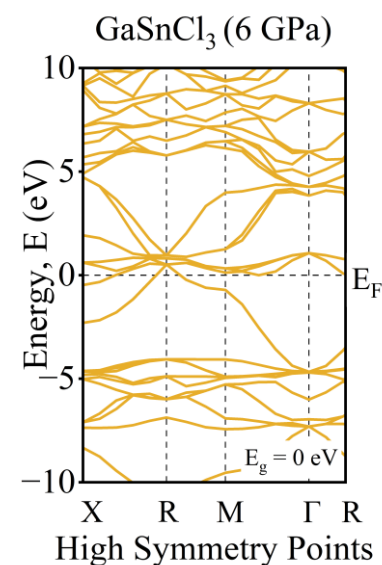
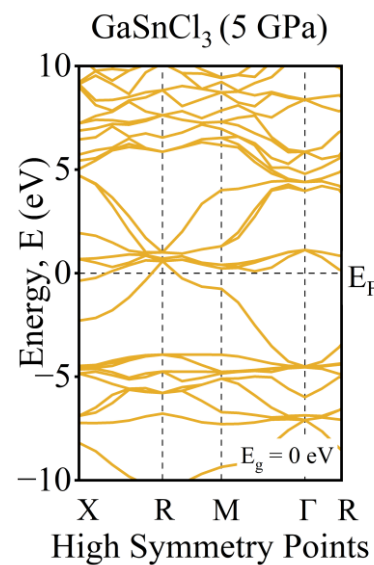
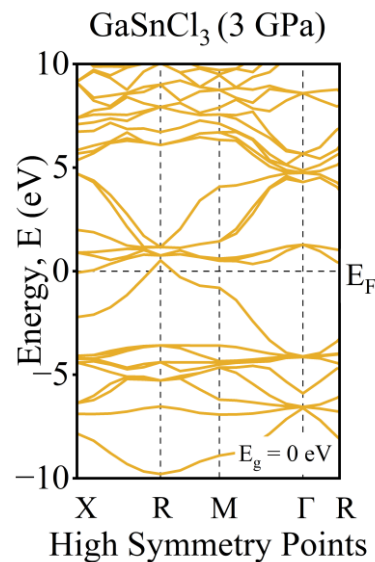
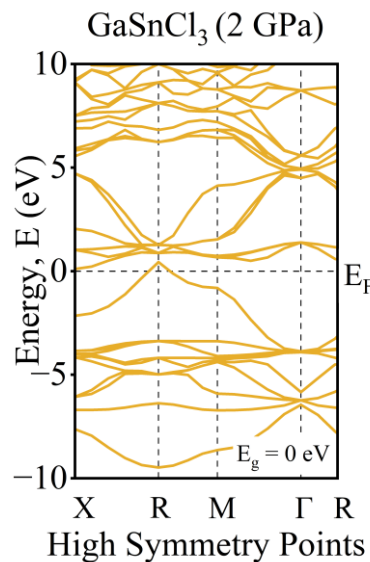
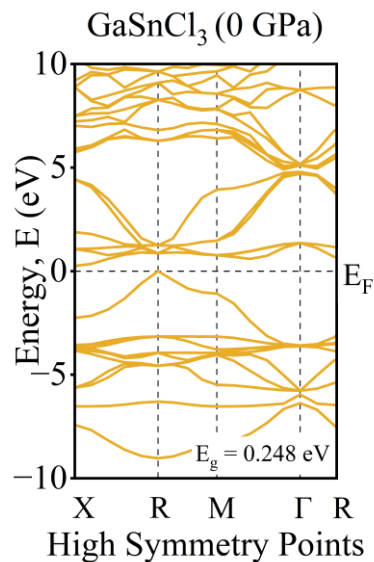
<sup>b</sup> Department of Electrical and Electronic Engineering, Bangladesh Army University of Science and Technology (BAUST), Saidpur-5311, Bangladesh.

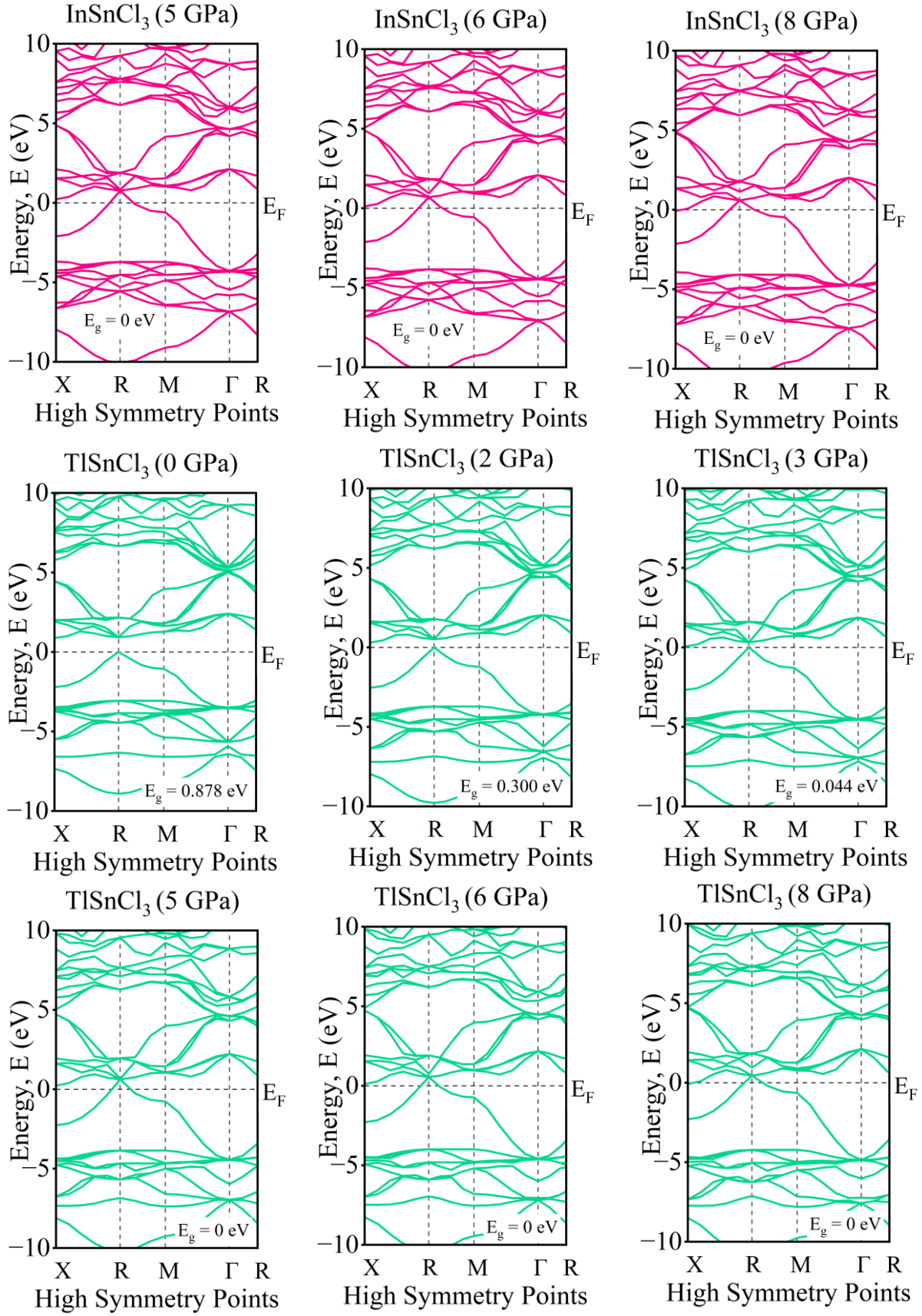
<sup>c</sup> Department of Materials and Metallurgical Engineering, Bangladesh University of Engineering and Technology (BUET), Dhaka-1000, Bangladesh.

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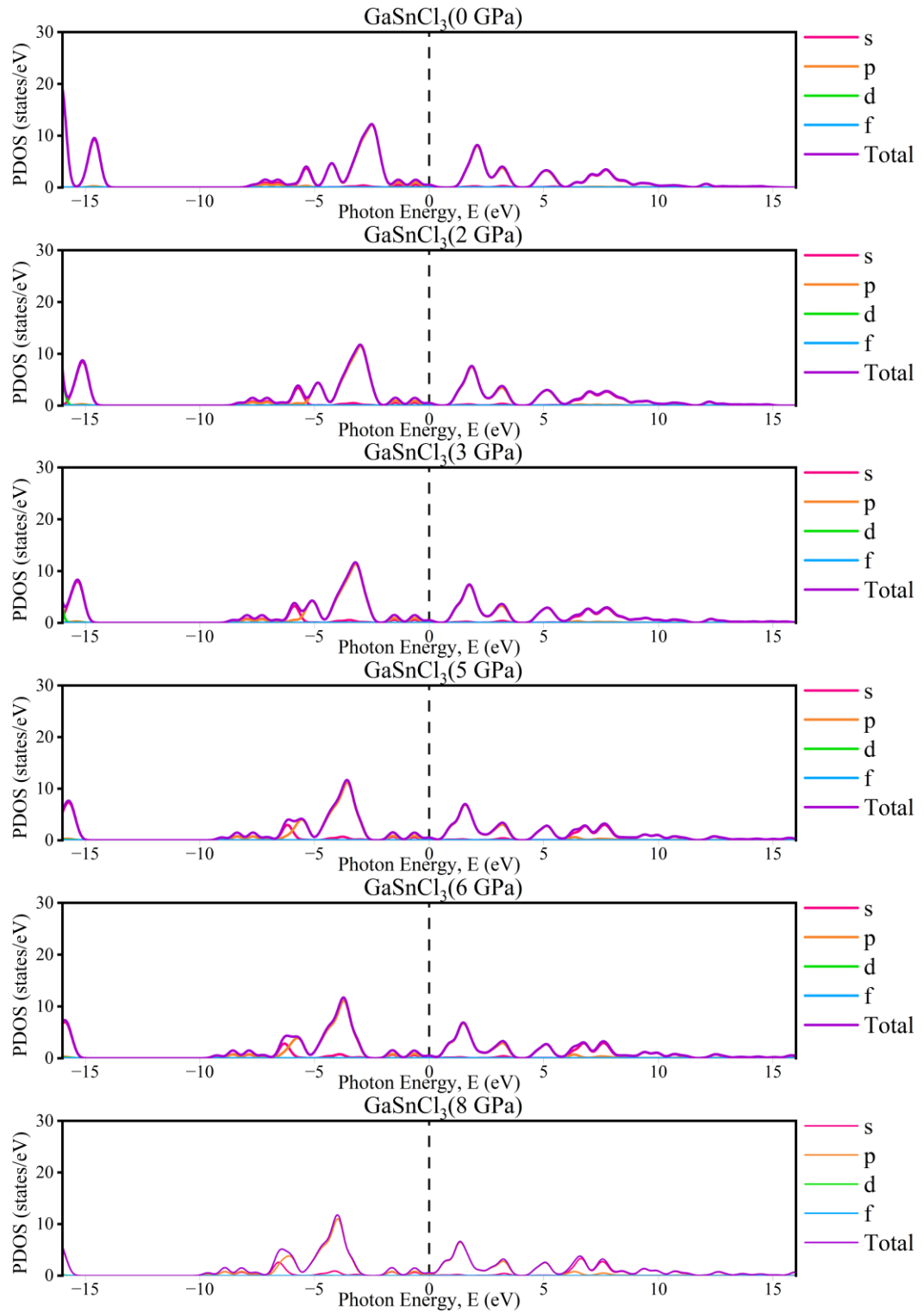
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GaSnCl<sub>3</sub> (0 GPa) GGA-PBeSOIGaSnCl<sub>3</sub> (0 GPa) mGGAInSnCl<sub>3</sub> (0 GPa) GGA-PBeSOIInSnCl<sub>3</sub> (0 GPa) mGGATlSnCl<sub>3</sub> (0 GPa) GGA-PBeSOITlSnCl<sub>3</sub> (0 GPa) mGGA

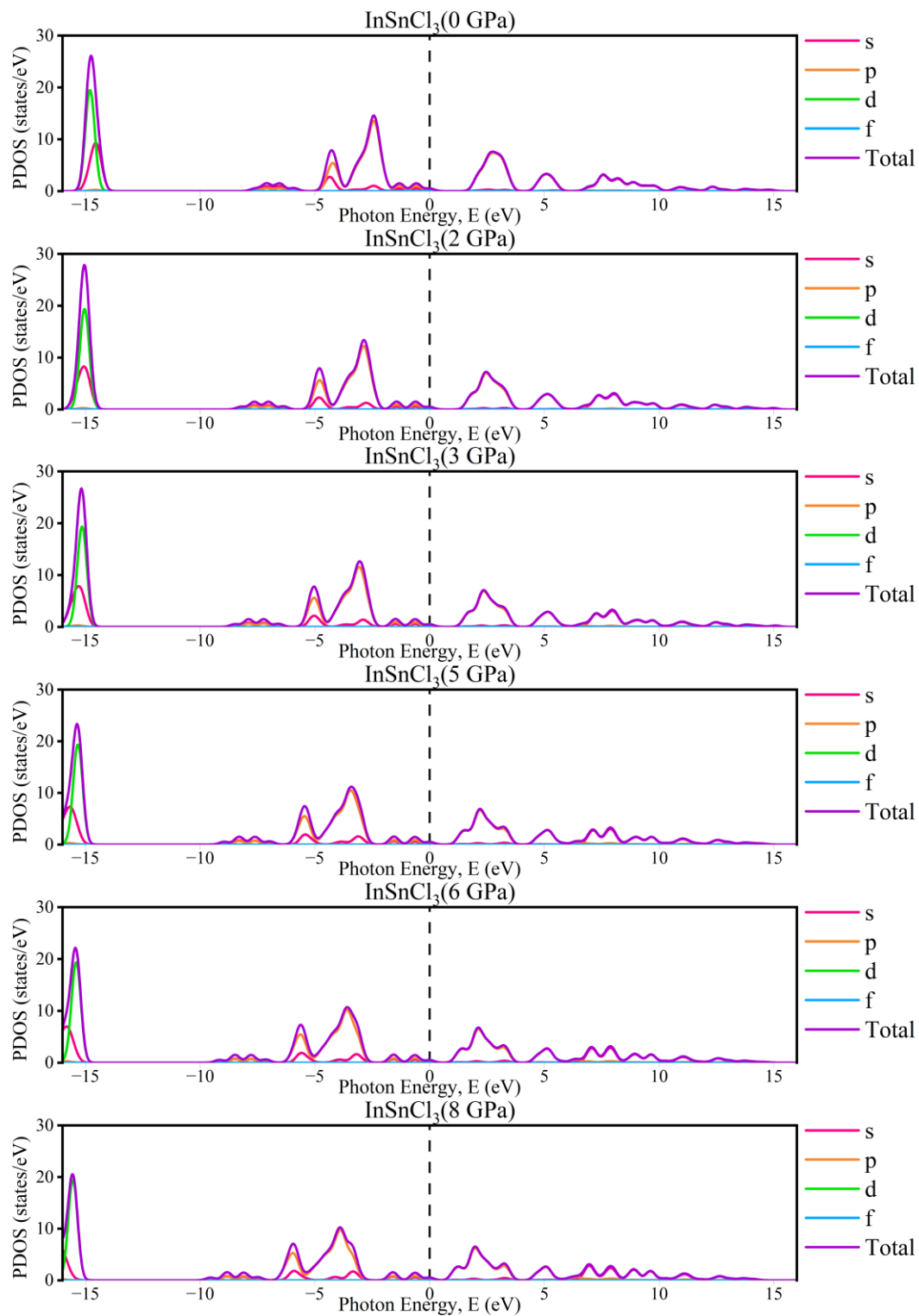




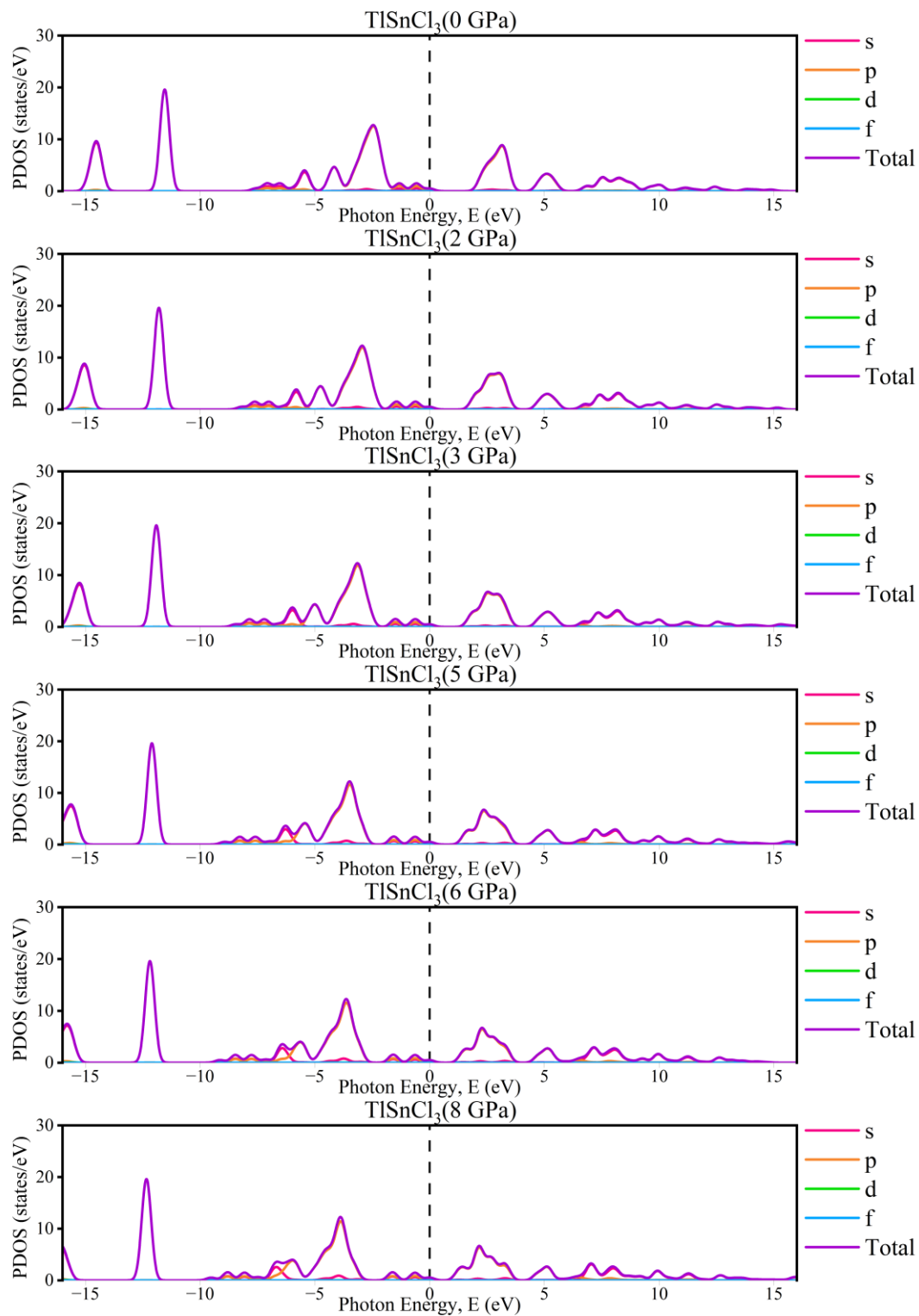
**Fig. 3.** Band structure of  $\text{ASnCl}_3$  ( $A = \text{Ga}, \text{In}, \text{and Tl}$ ) under pressure.



**Fig. 5.** The Partial Density of States (PDOS) of  $\text{ASnCl}_3$  ( $A = \text{Ga}, \text{In}, \text{and Tl}$ ) under pressure.



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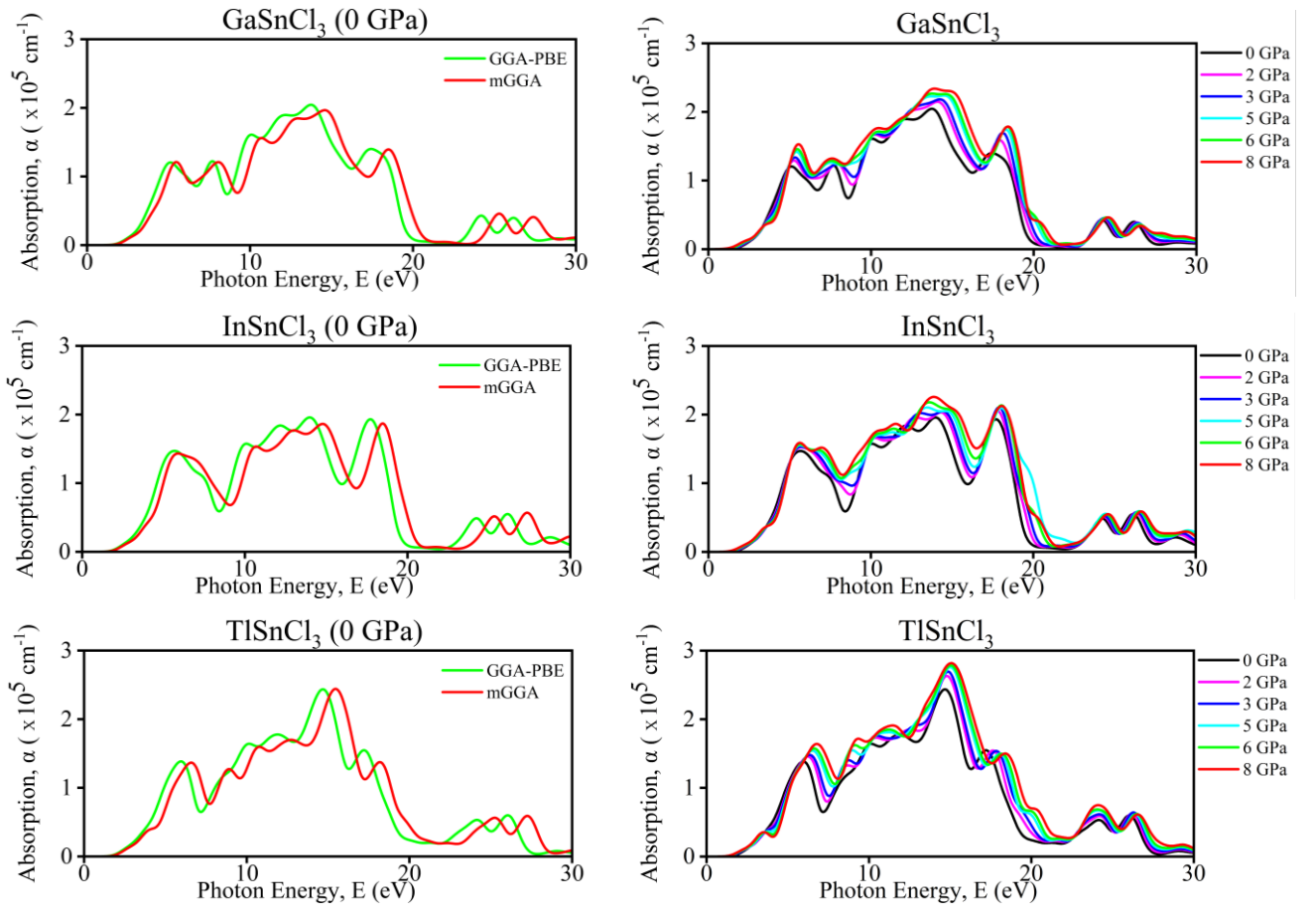
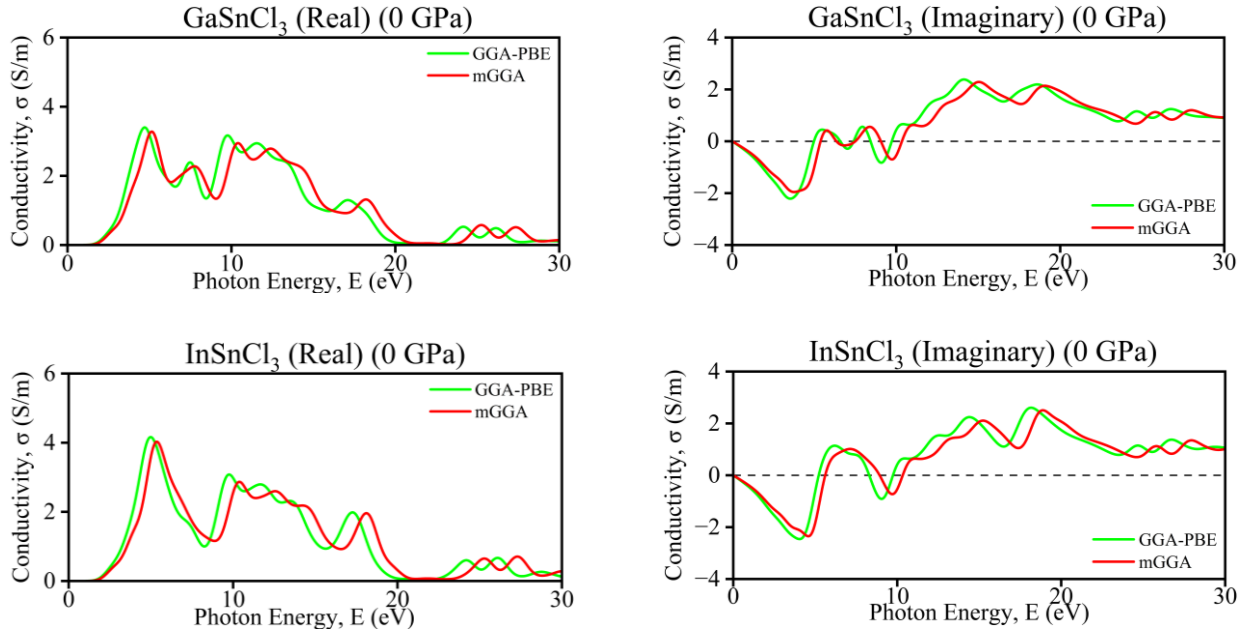
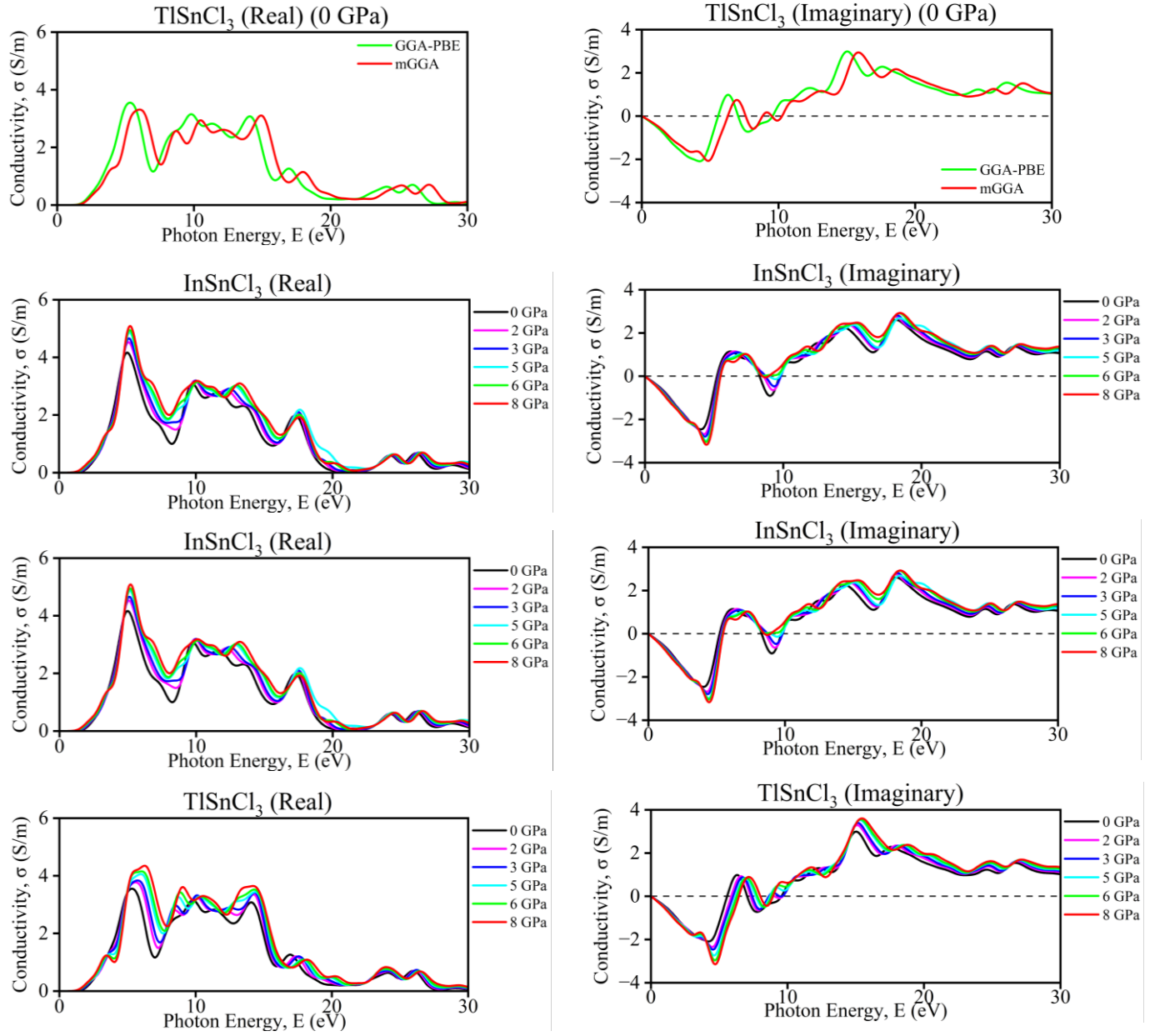


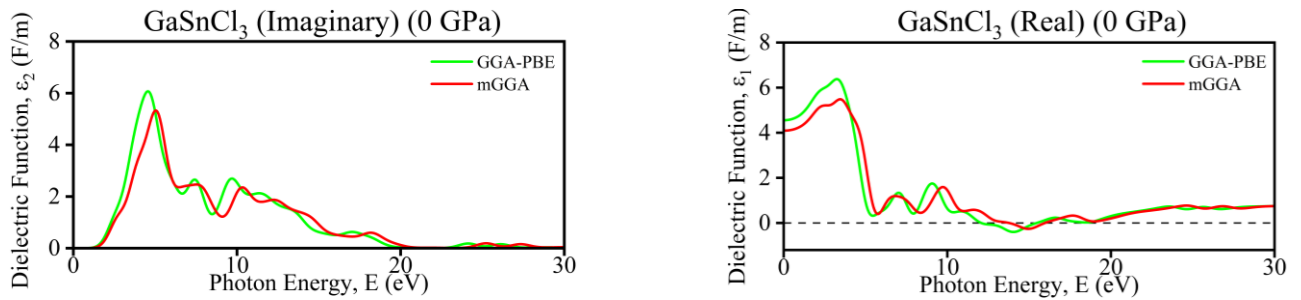
Fig. 7. Calculated pressure-induced spectra of absorption ( $\alpha$ ) for  $\text{ASnCl}_3$  ( $A = \text{Ga, In, and Tl}$ ).

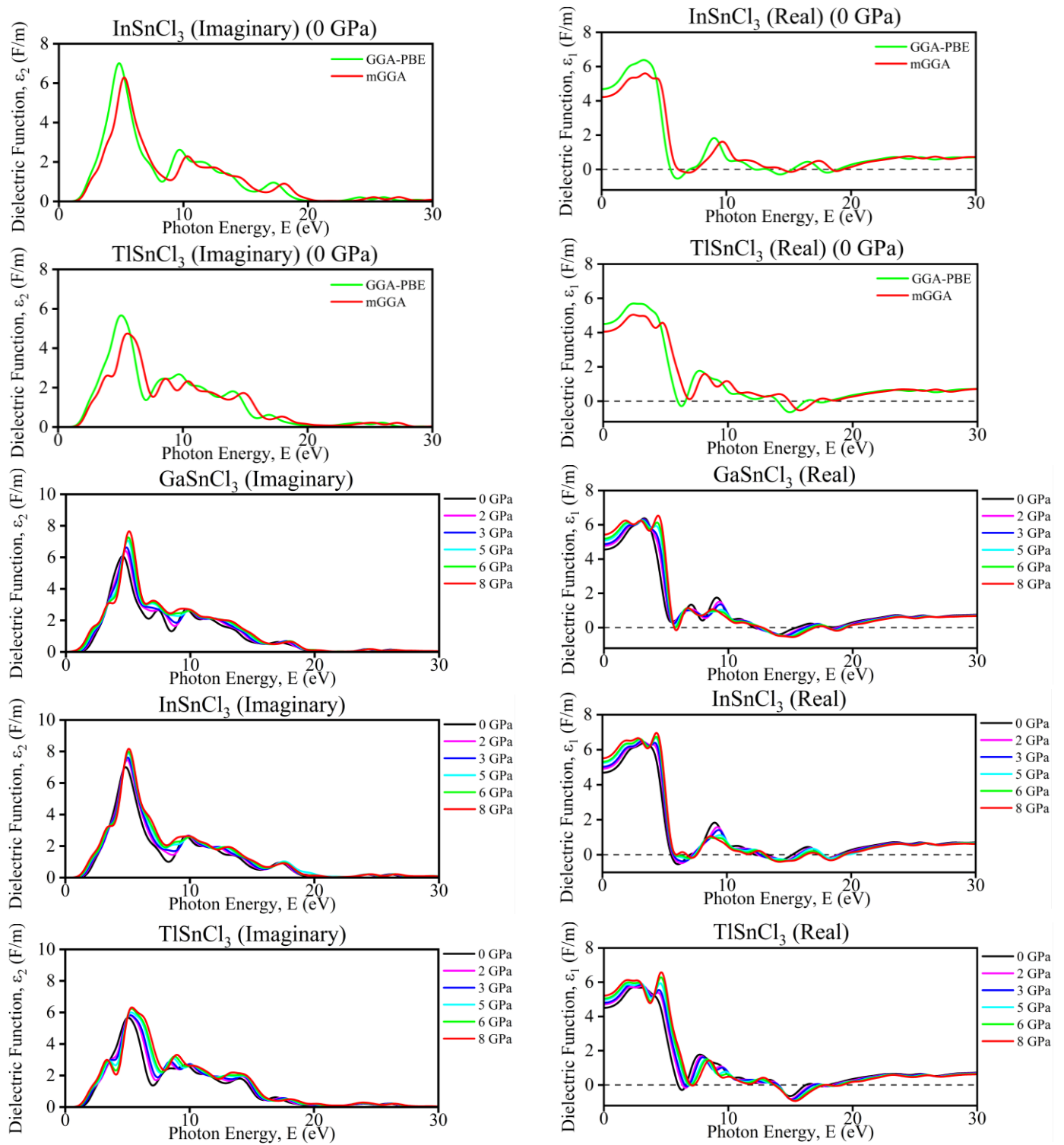




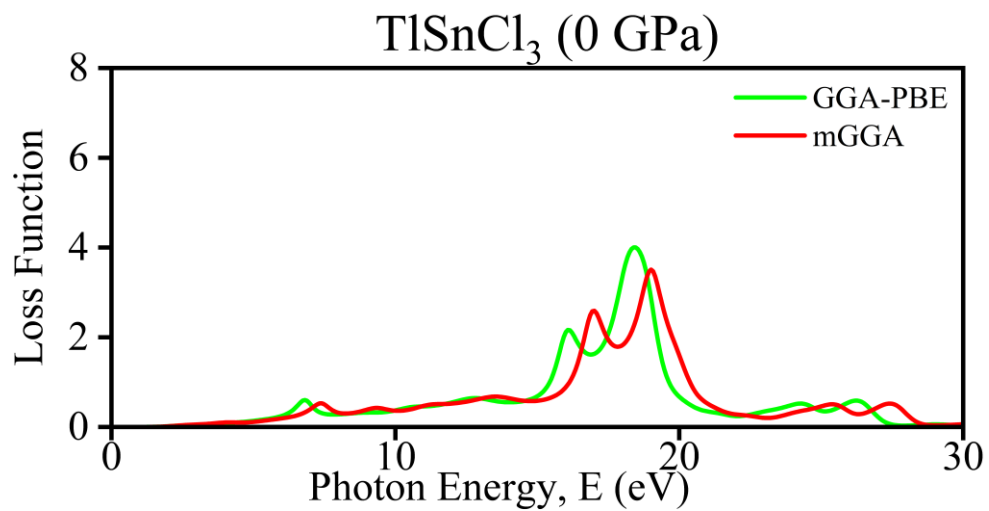
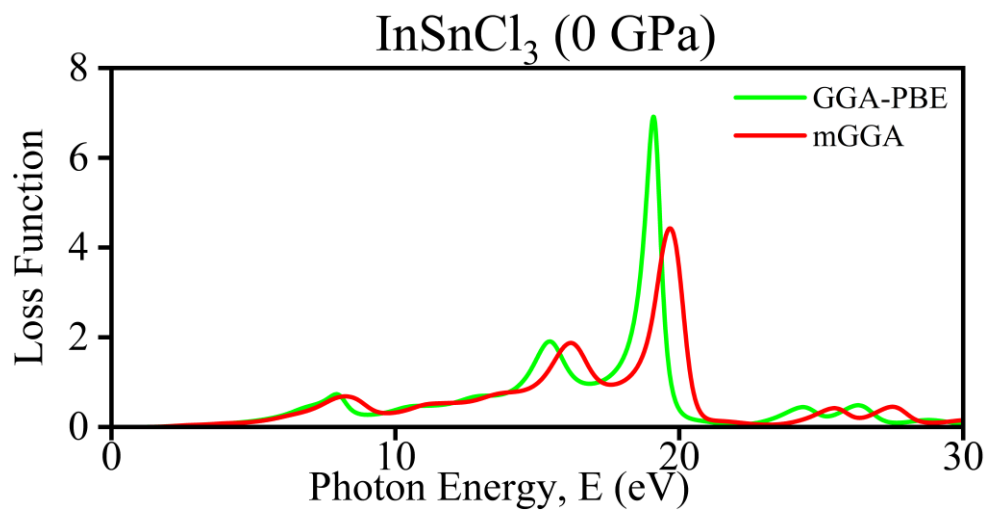
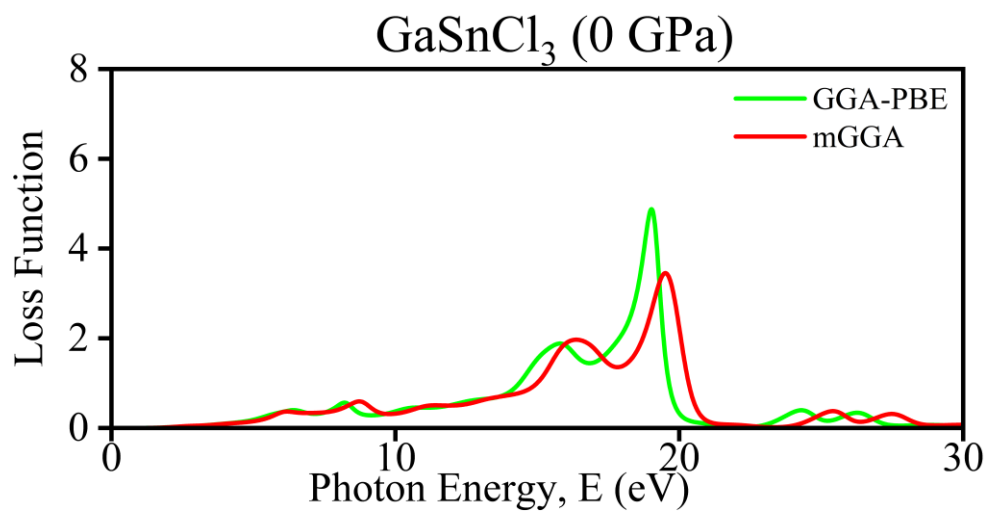


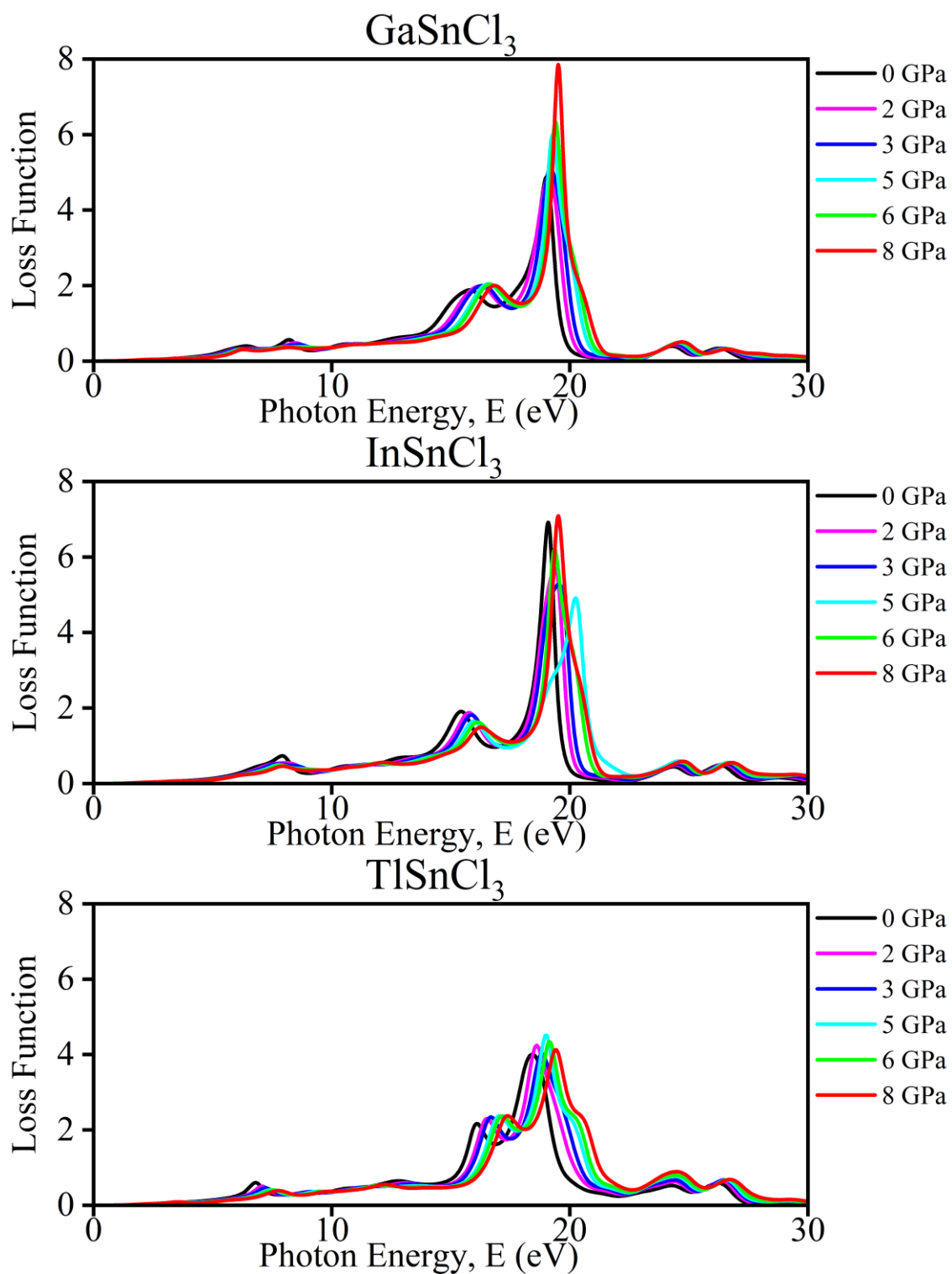
**Fig. 8.** Calculated pressure-induced Imaginary and real spectra of optical conductivity ( $\sigma$ ) for  $\text{ASnCl}_3$  ( $A = \text{Ga}, \text{In}, \text{and Tl}$ ).



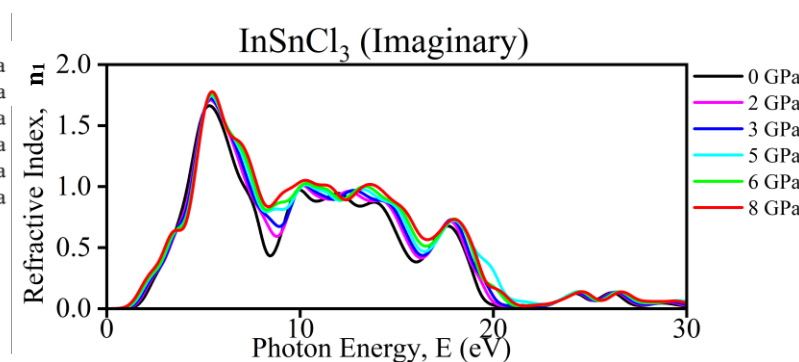
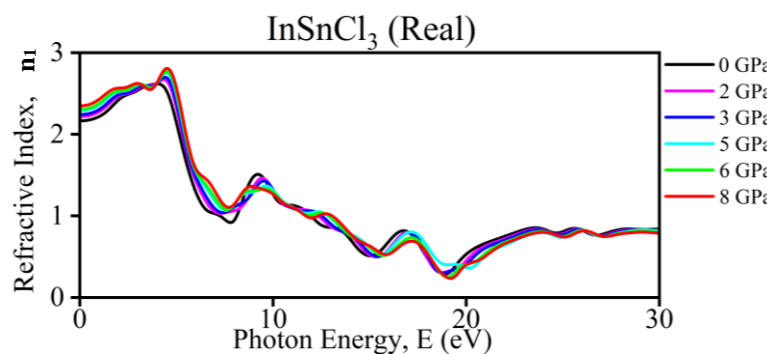
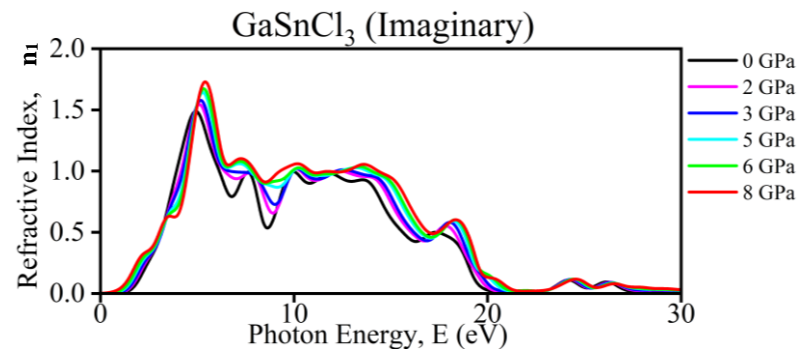
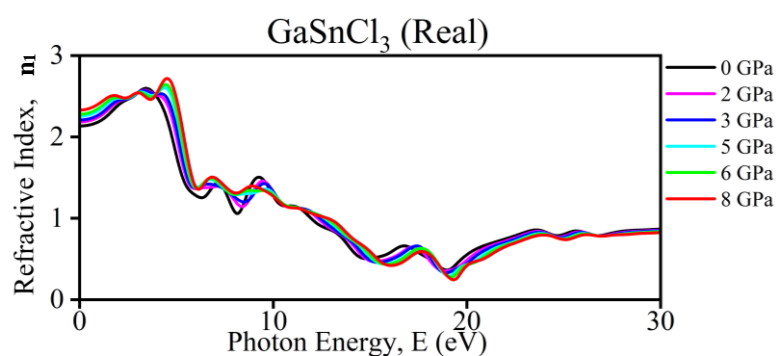
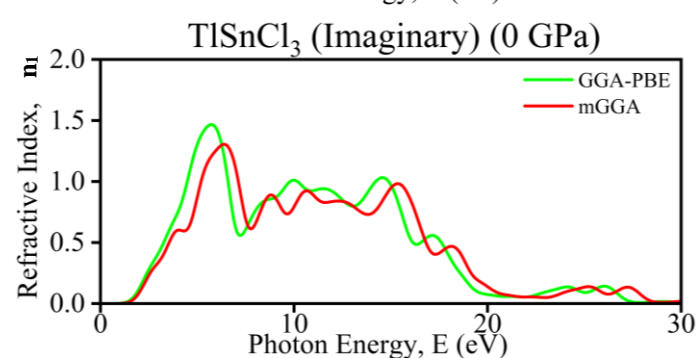
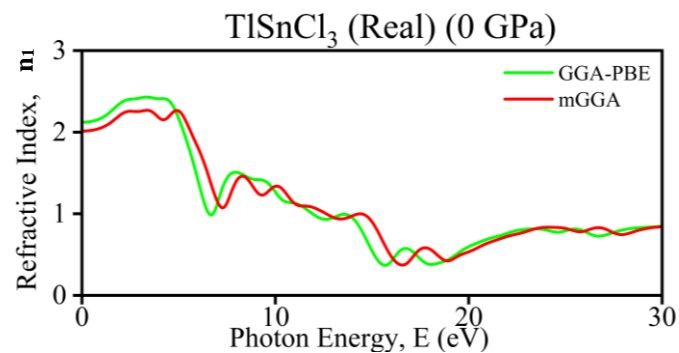
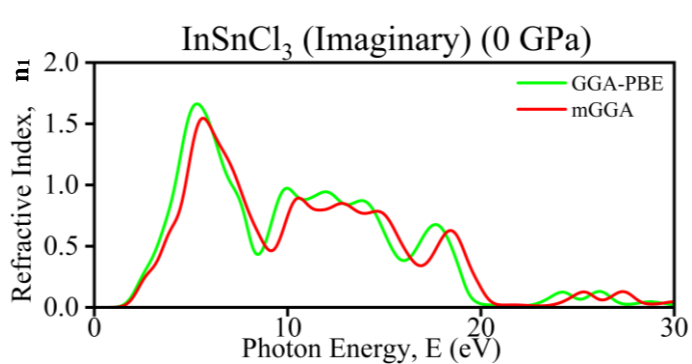
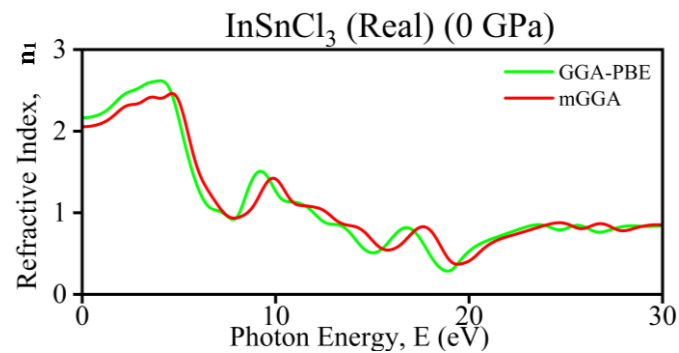
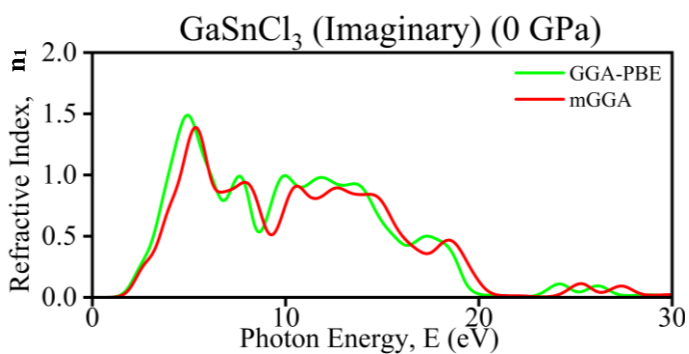
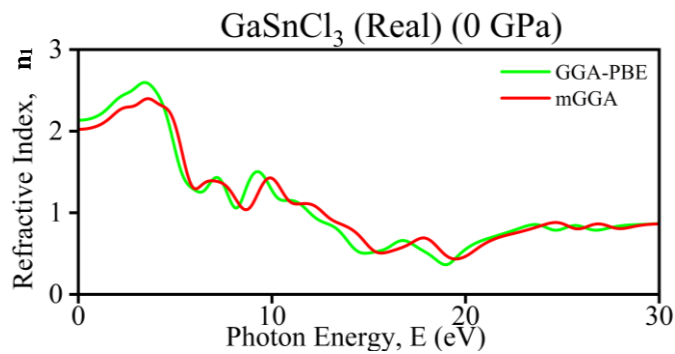


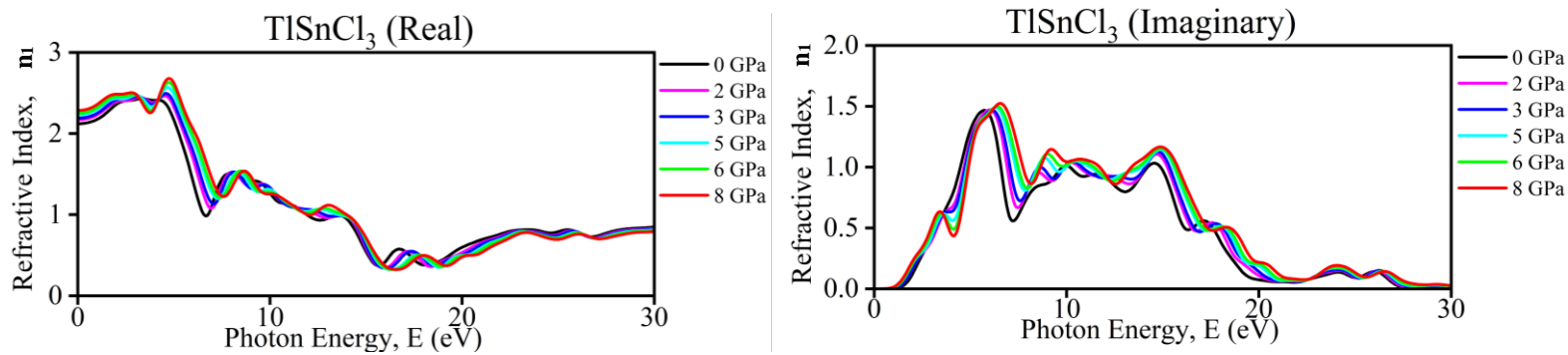
**Fig. 9. & 10.** Calculated pressure induced imaginary spectra & real spectra of dielectric function ( $\epsilon$ ) for  $\text{ASnCl}_3$  ( $A = \text{Ga}, \text{In}, \text{and Tl}$ ).





**Fig. 11.** Calculated pressure-induced spectra of loss function of  $\text{ASnCl}_3$  ( $A = \text{Ga}, \text{In}, \text{and Tl}$ ).





**Fig. 12.** Calculated pressure induced spectra of the Refractive index ( $n_1$ ) of  $\text{ASnCl}_3$  ( $A = \text{Ga}, \text{In},$  and  $\text{Tl}$ ).