

## Supplementary Information

### Correlation between band gap and Raman intensity

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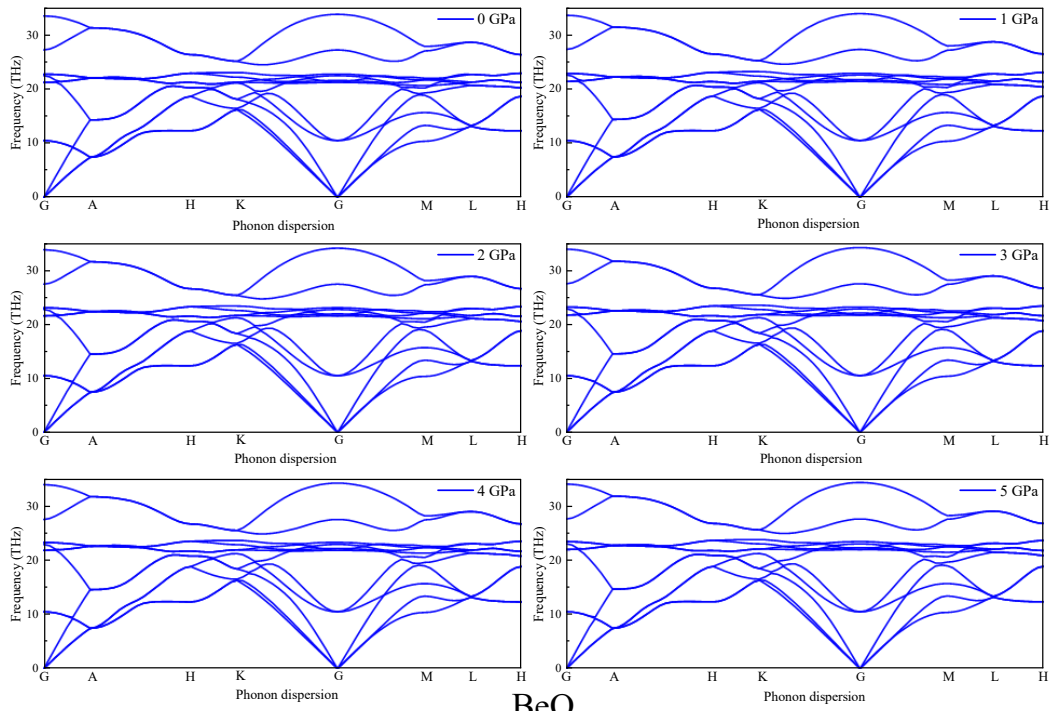
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This article mainly supplements some details and contents of the main text. Including the calculated phonon spectra under pressure from 0 to 5 GPa; the band structures under pressure from 0 to 5 GPa; the band structures of HgSe under pressure from 10 to 50 GPa.

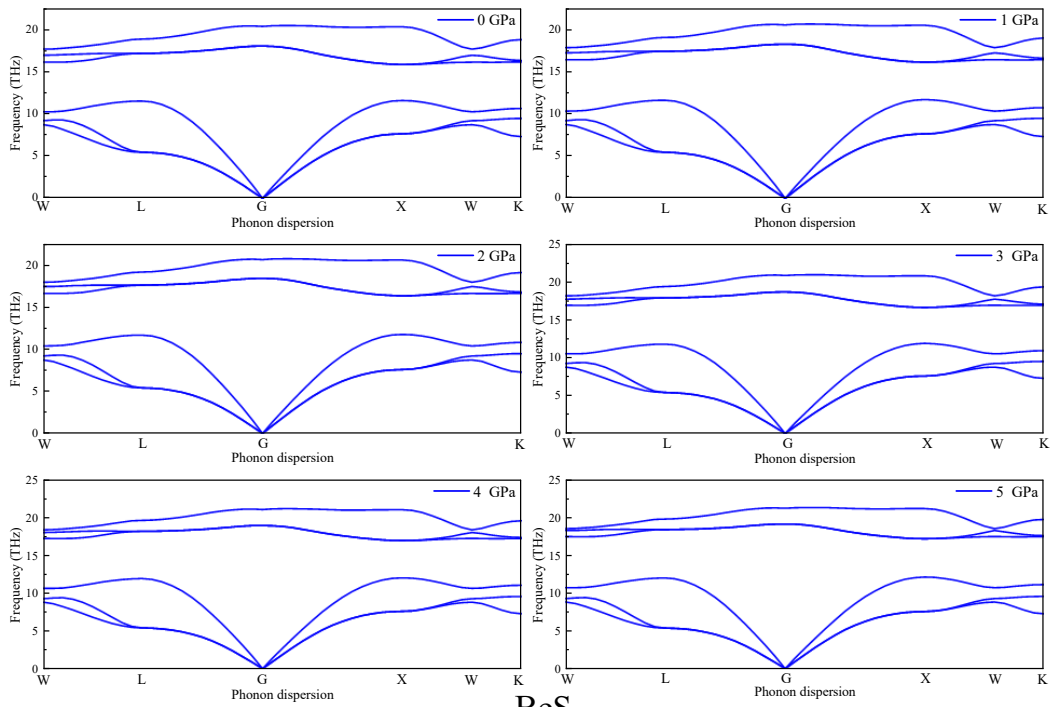
**The calculated phonon spectra under pressure from 0 to 5 GPa.** Figure S1 presents the complete phonon dispersion for all 18 structures in this study under pressures from 0 to 5 GPa. They can effectively demonstrate the vibration characteristics and kinetic stability of the structure, and are necessary calculations for verification before conducting further research.

**The band structures under pressure from 0 to 5 GPa.** Figure S2 shows the band structures of all 18 materials under pressures from 0 to 5 GPa. The main text only provided the band gap values for these materials. Although this does not affect the main discussion, we still choose to provide all the band structures in this SI section, as this can offer readers more specific information.

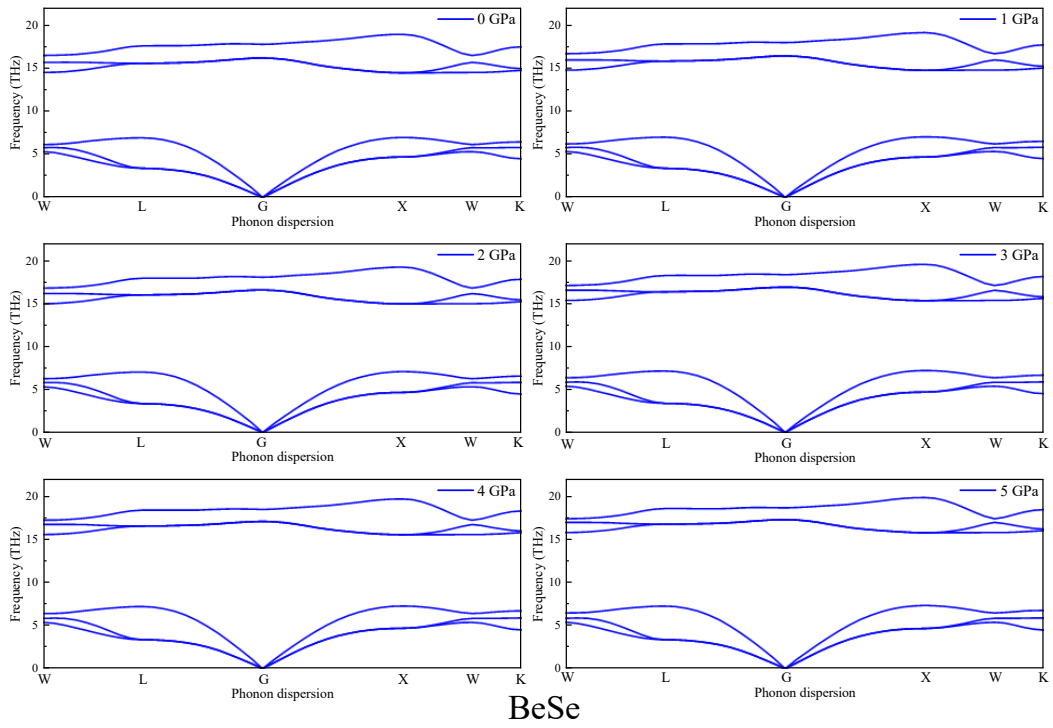
**The band structures of HgSe under pressure from 10 to 50 GPa.** The Raman intensity of HgSe decreases as the pressure increases, but its band gap does not open within 5 GPa. To verify the trend of the band gap change at higher pressures, we calculated the band structures of HgSe at higher pressure. As can be seen from Figure S3, its band gap opens at 40 GPa.



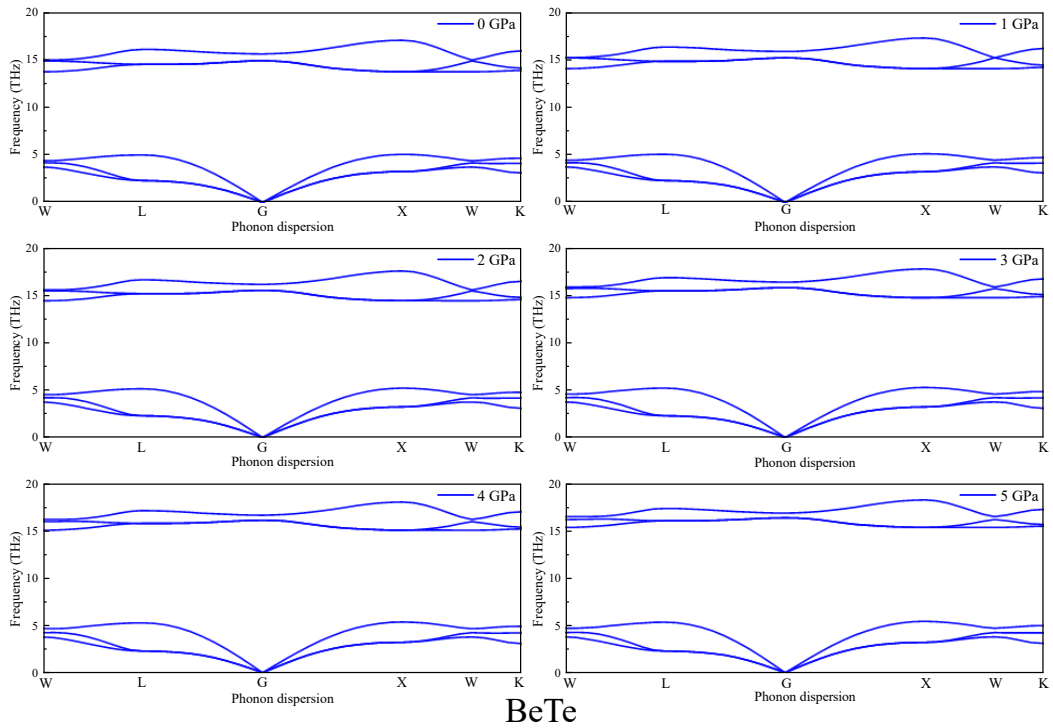
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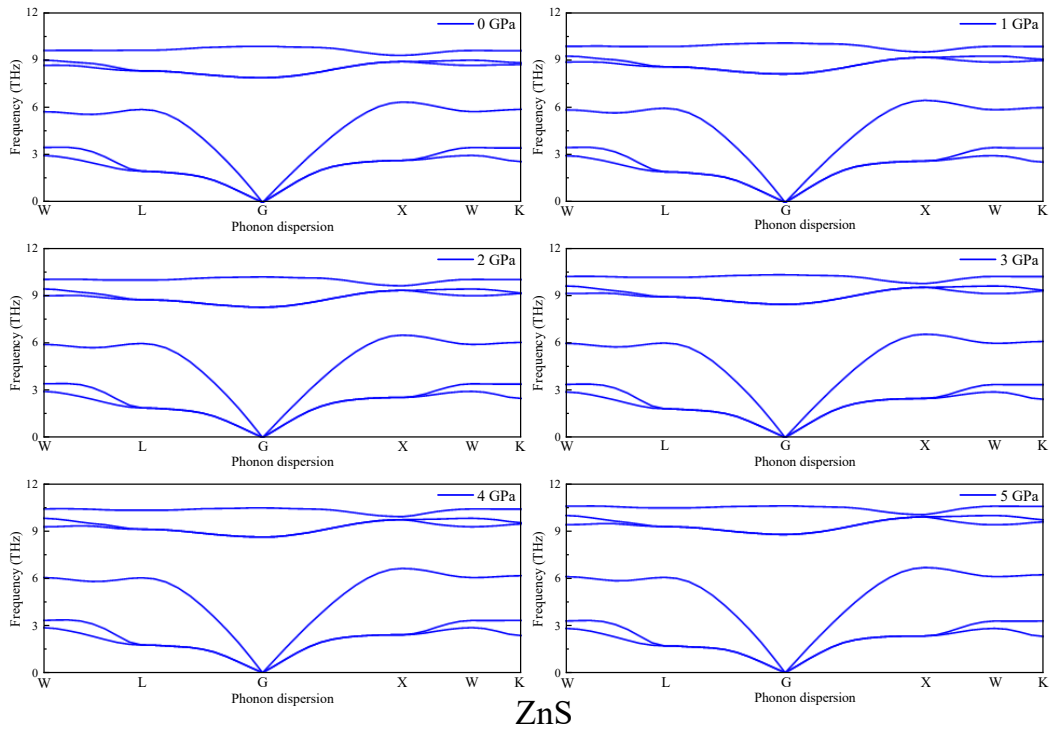
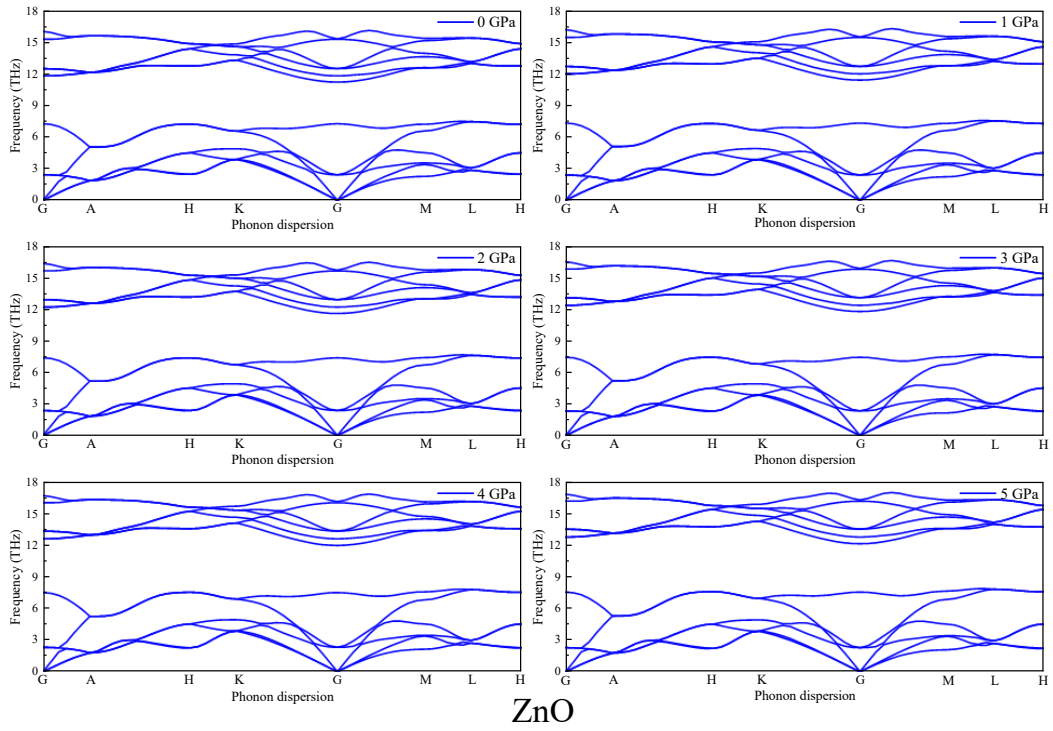
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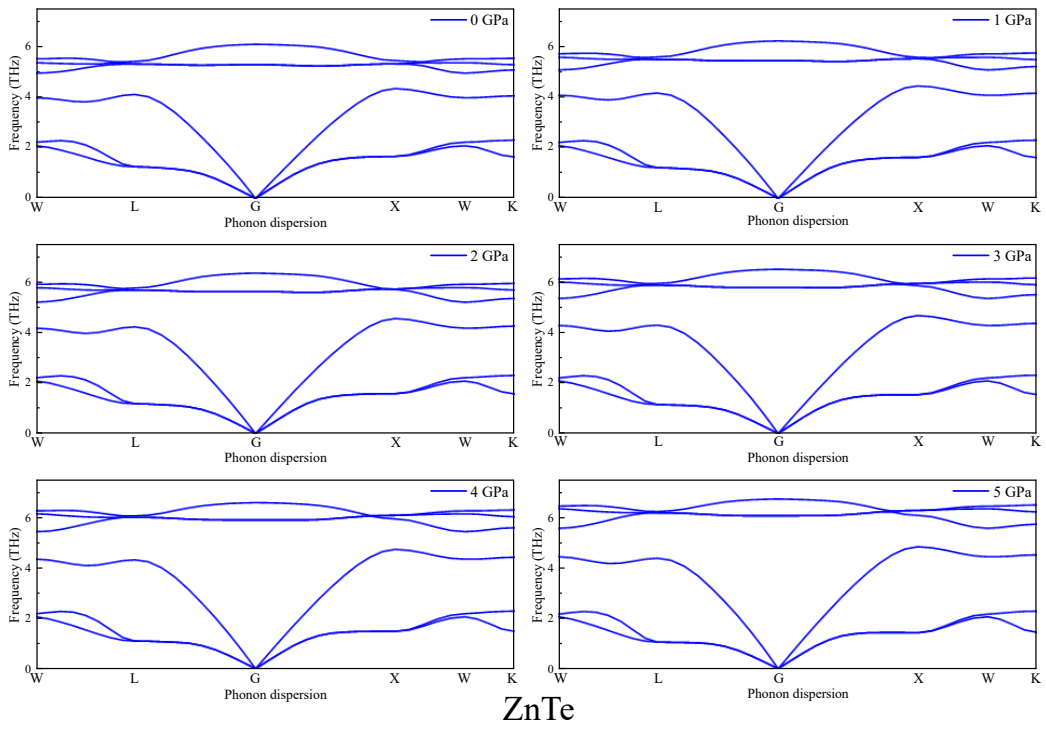
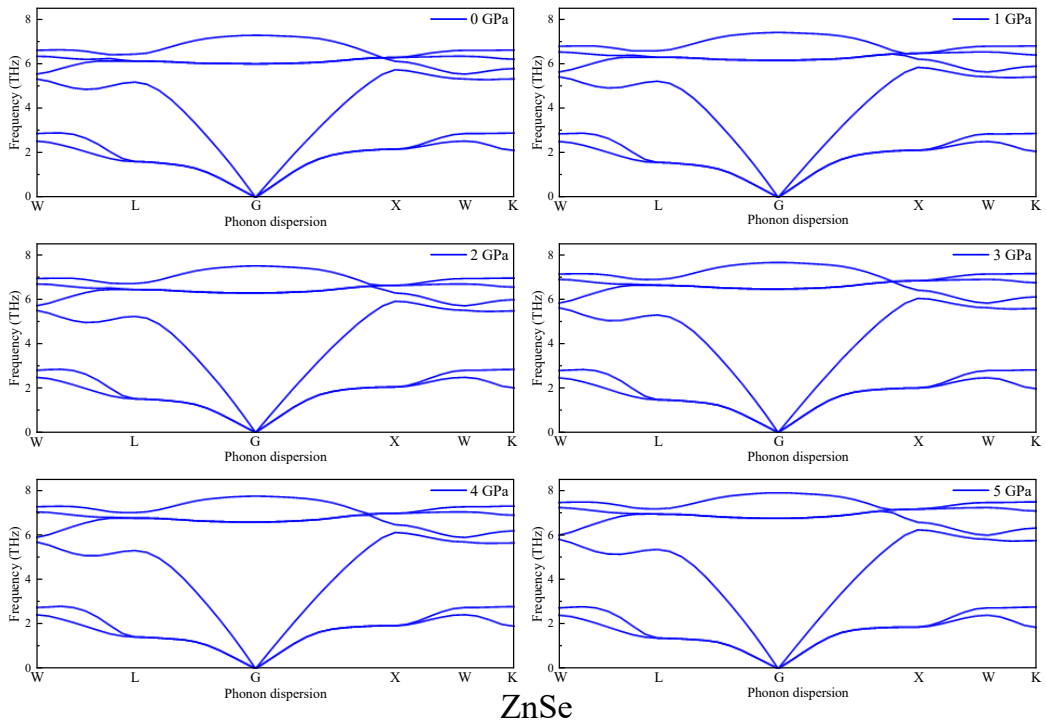


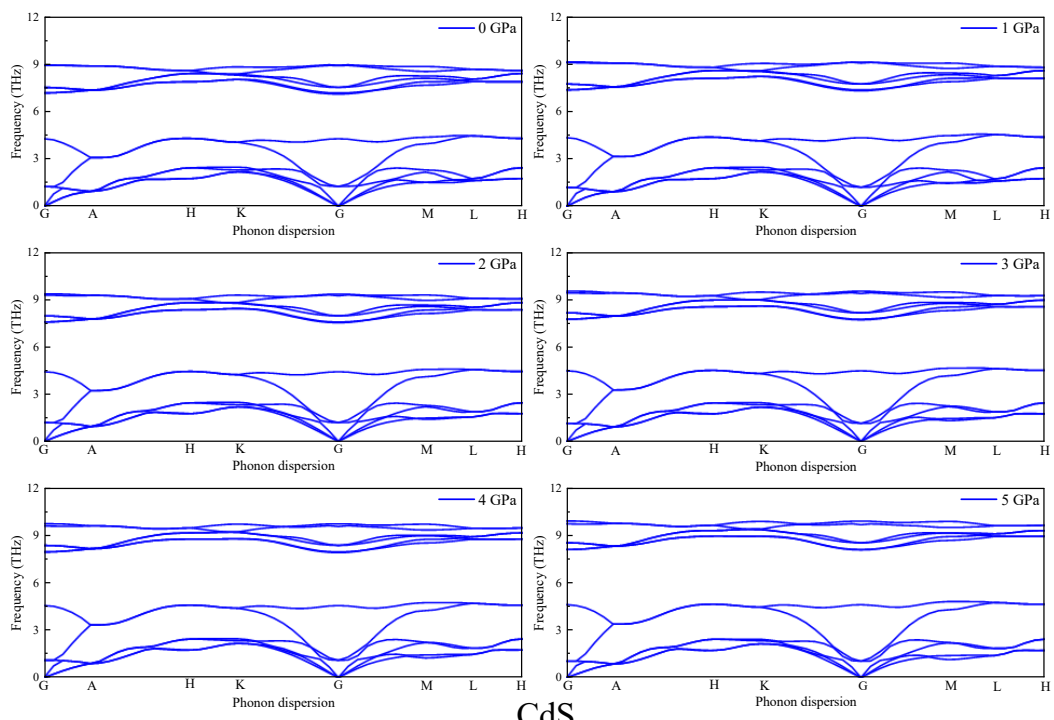
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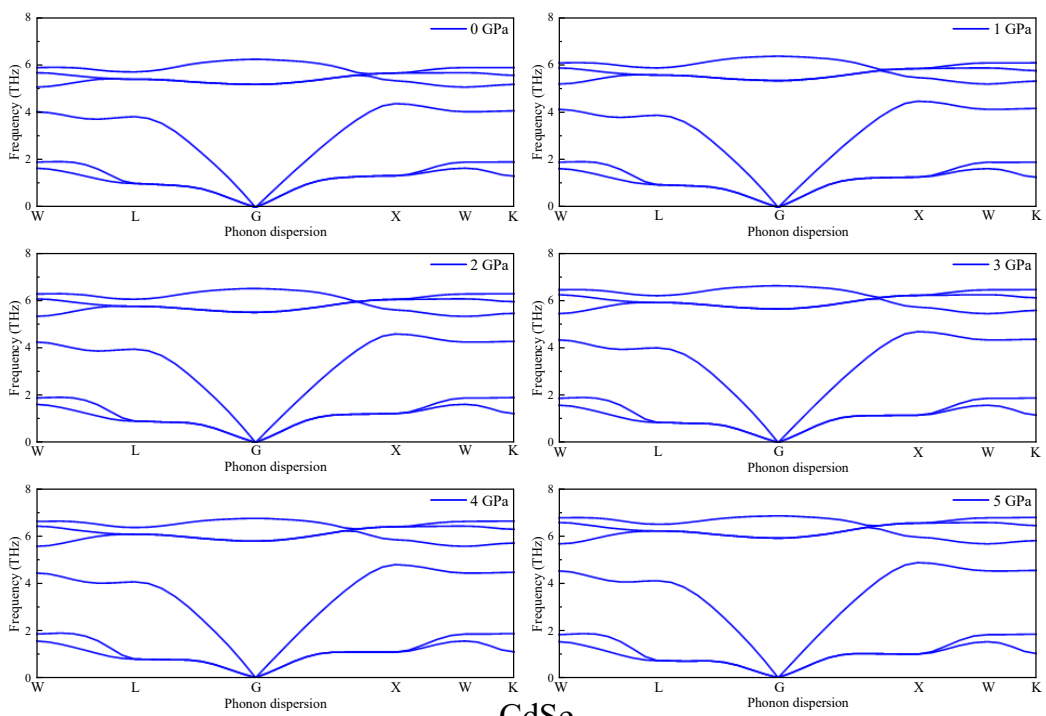
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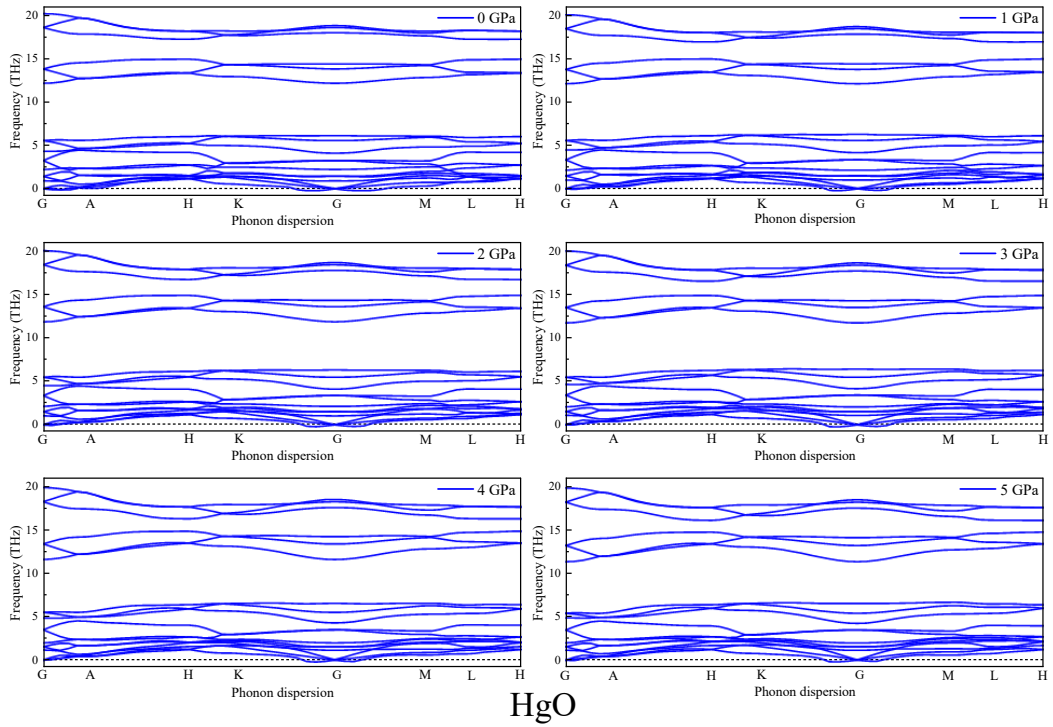
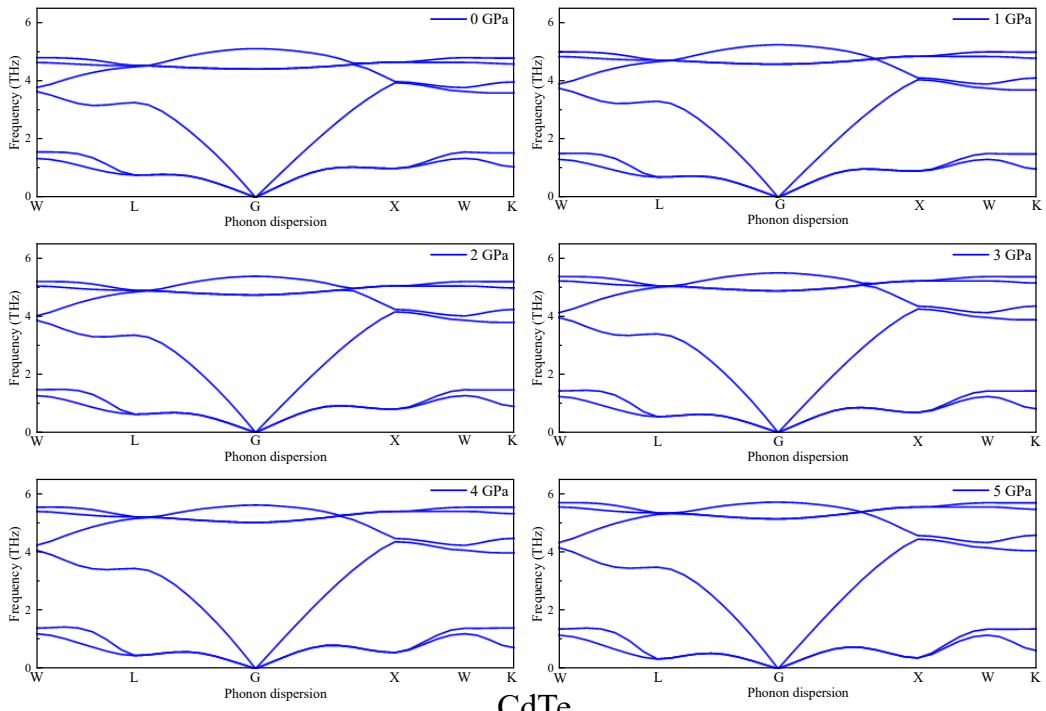


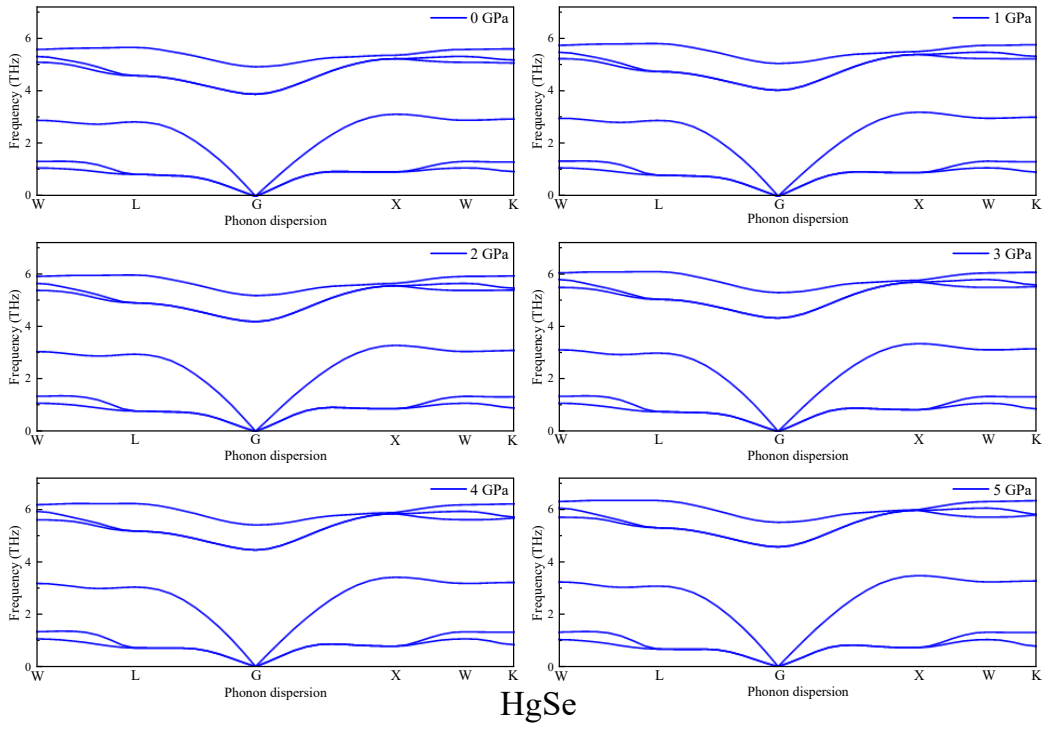
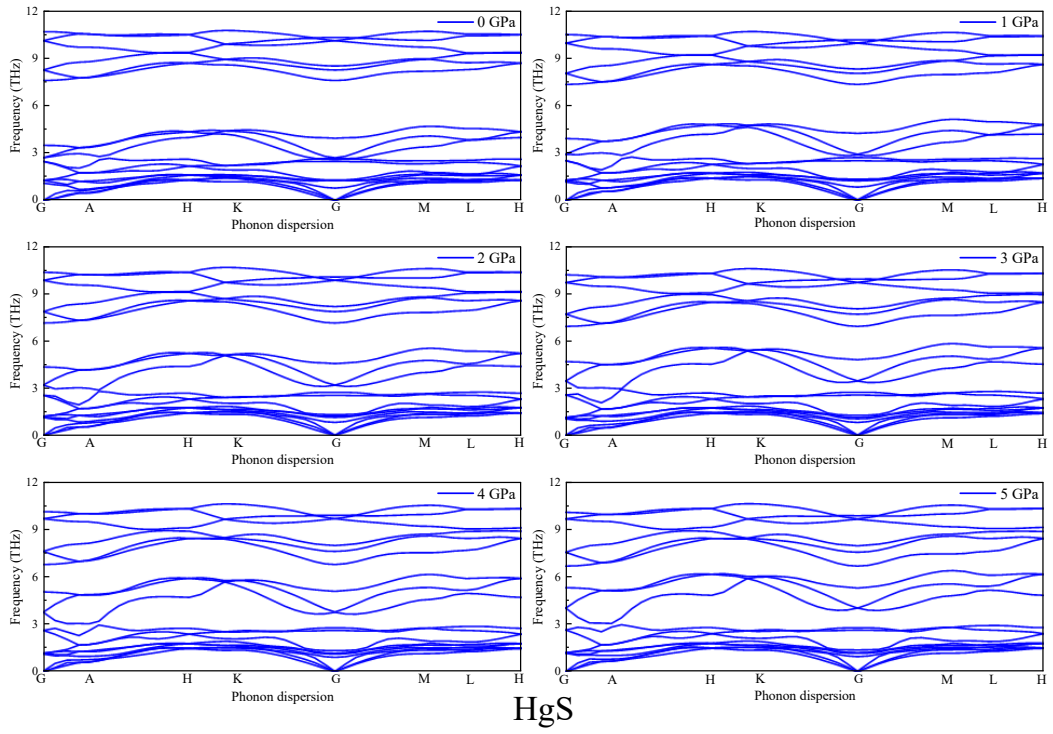


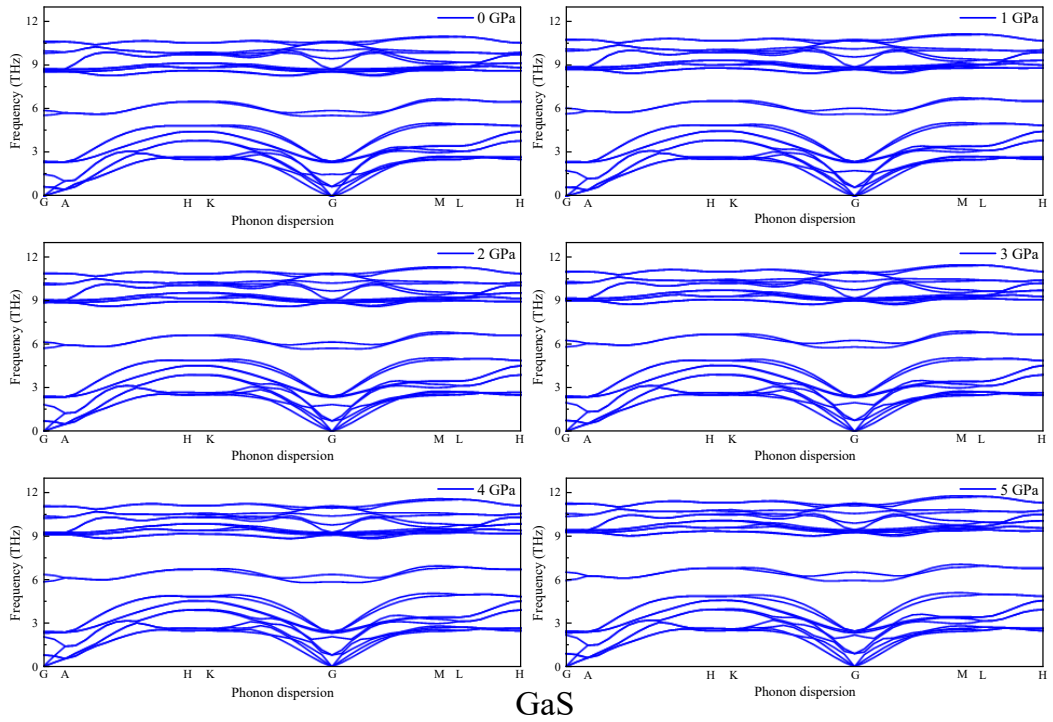
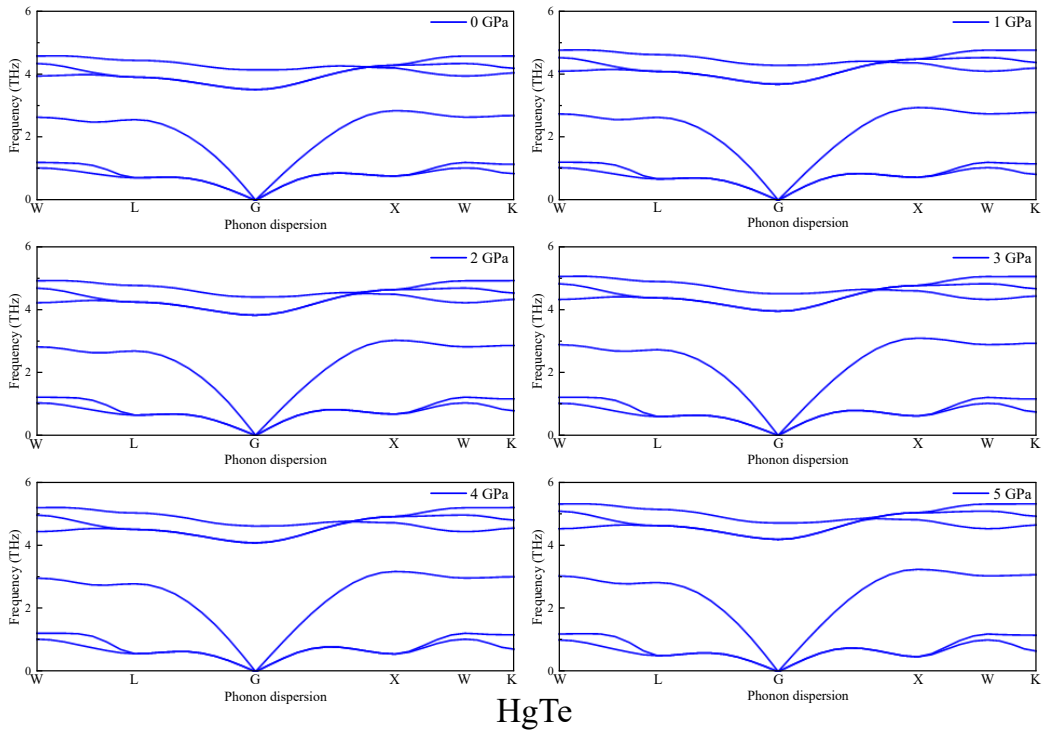
CdS



CdSe







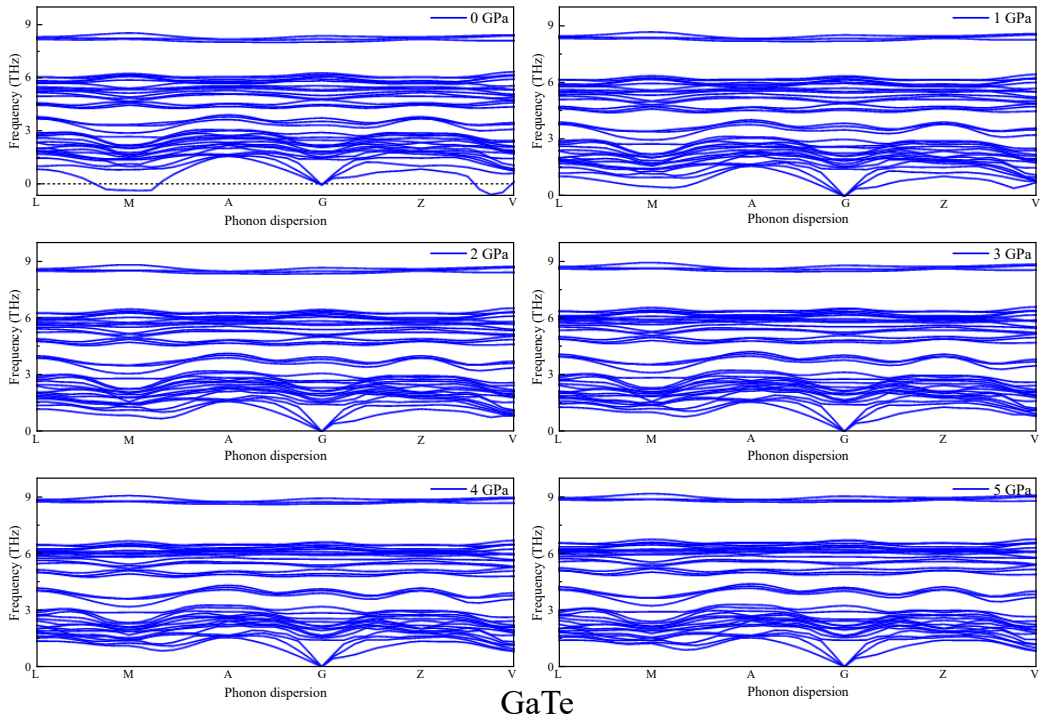
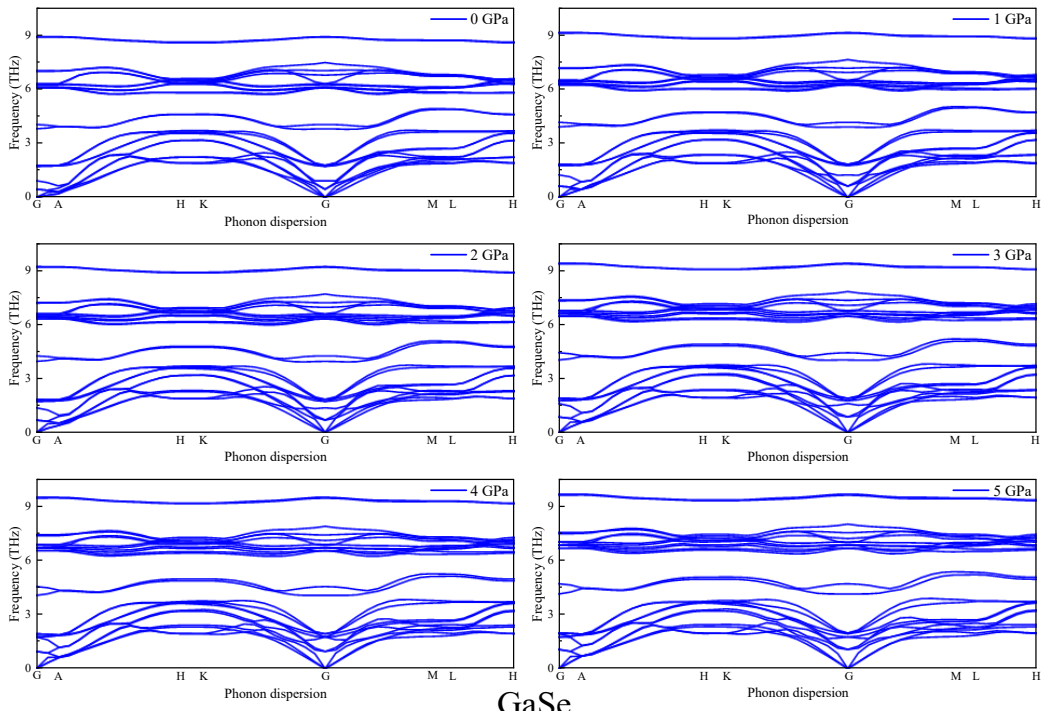
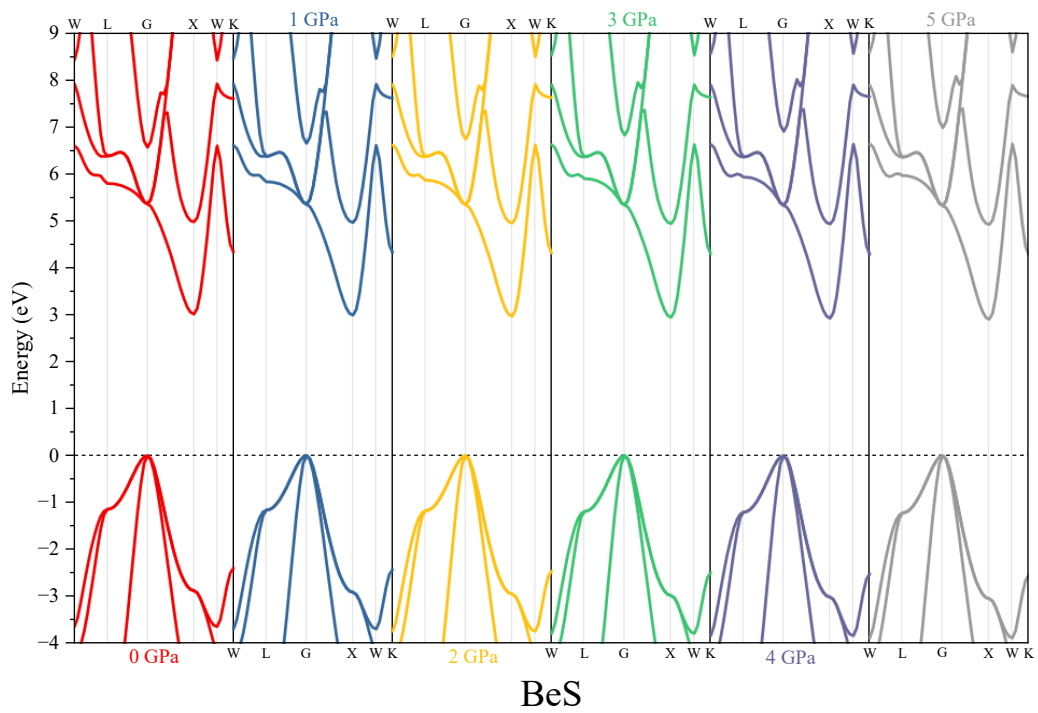
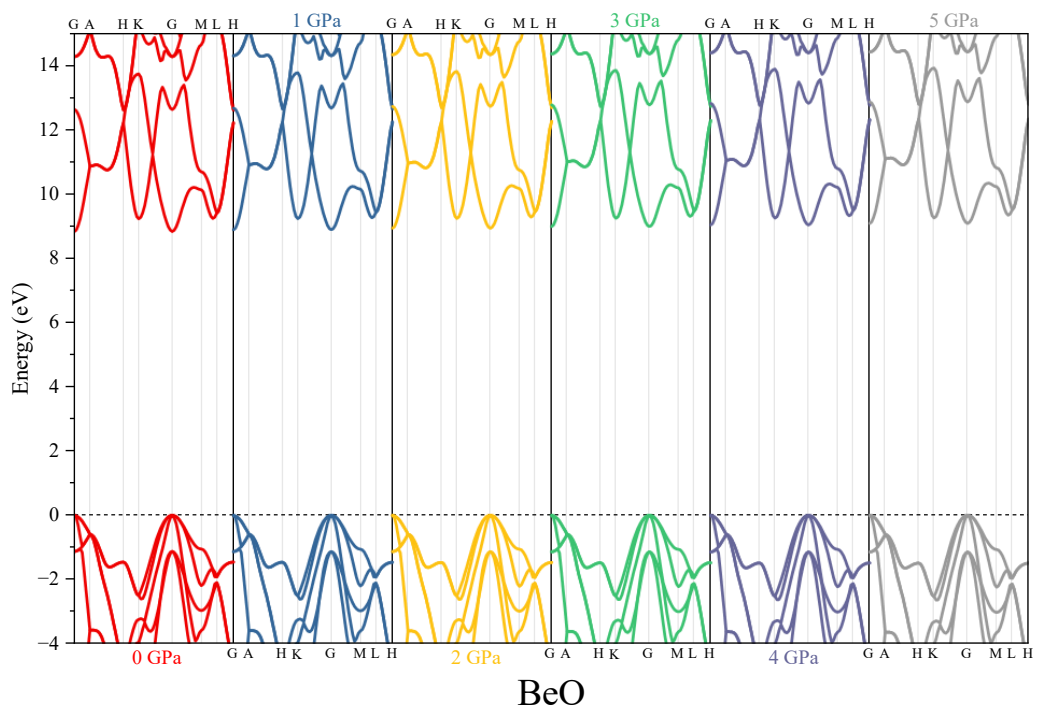
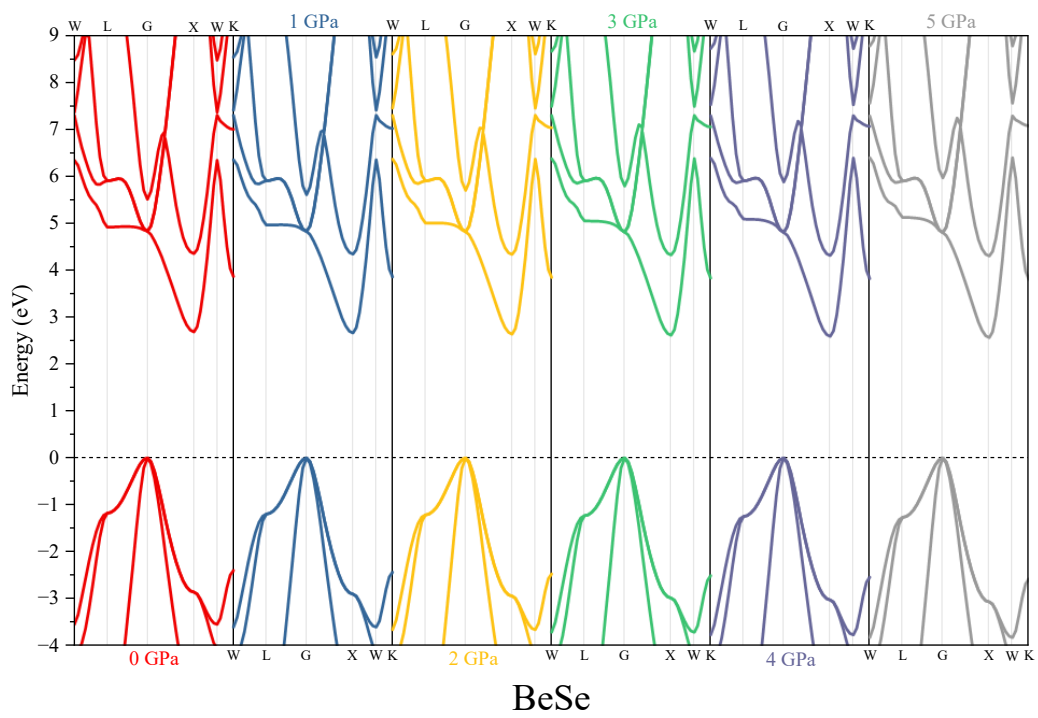
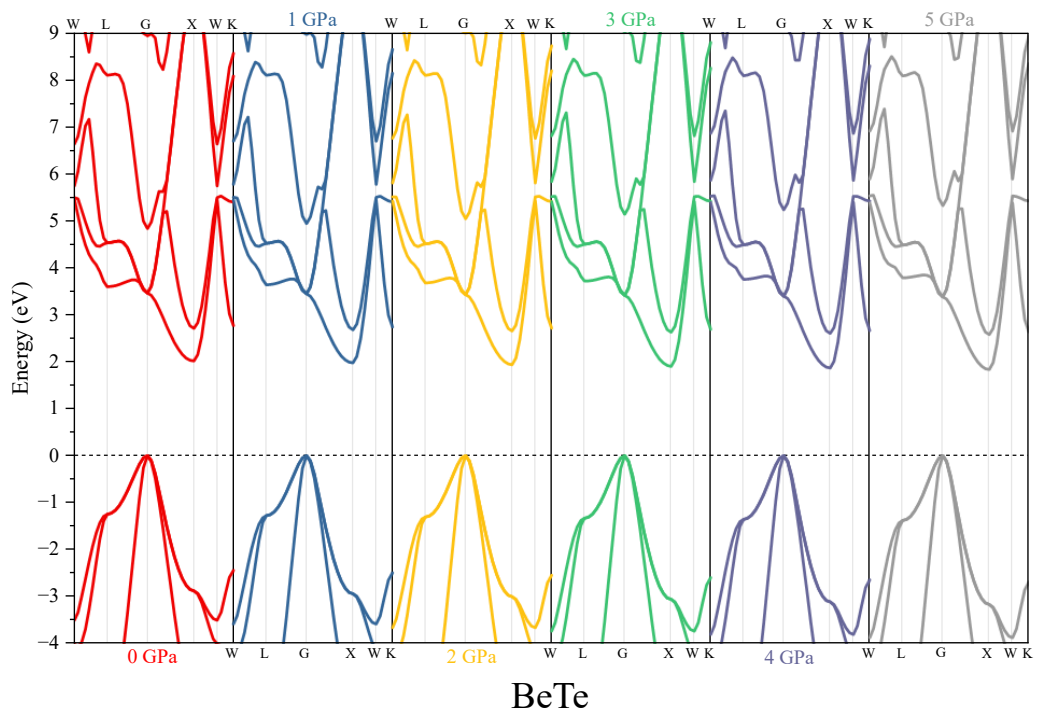


FIG. S1. The calculated phonon spectra under pressure from 0 to 5 GPa.

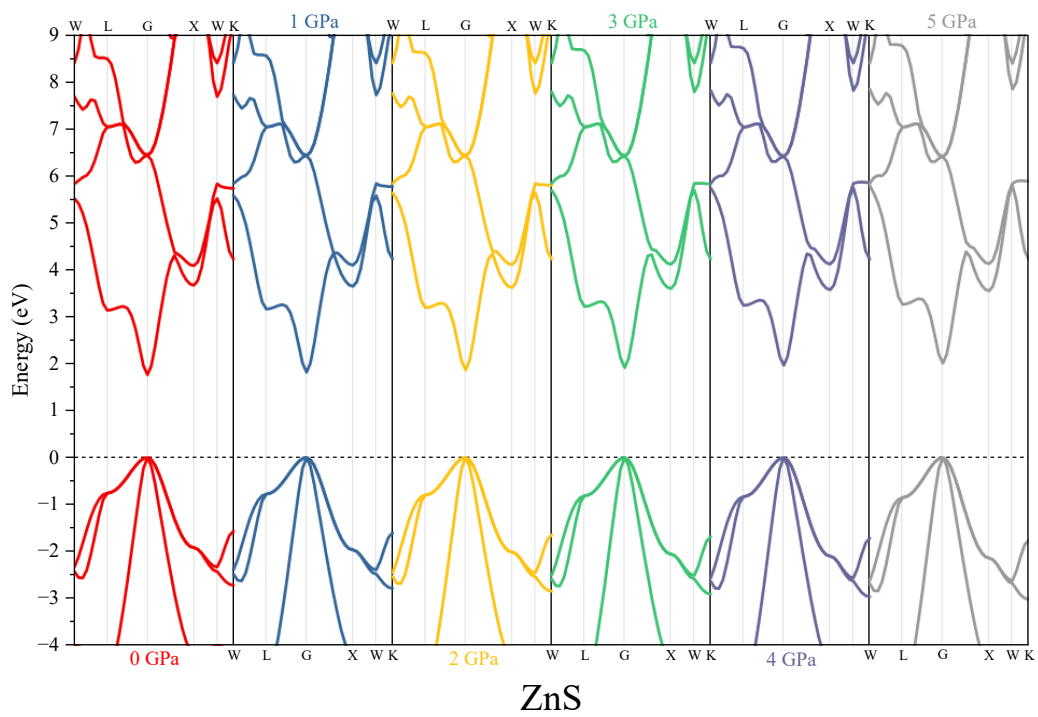
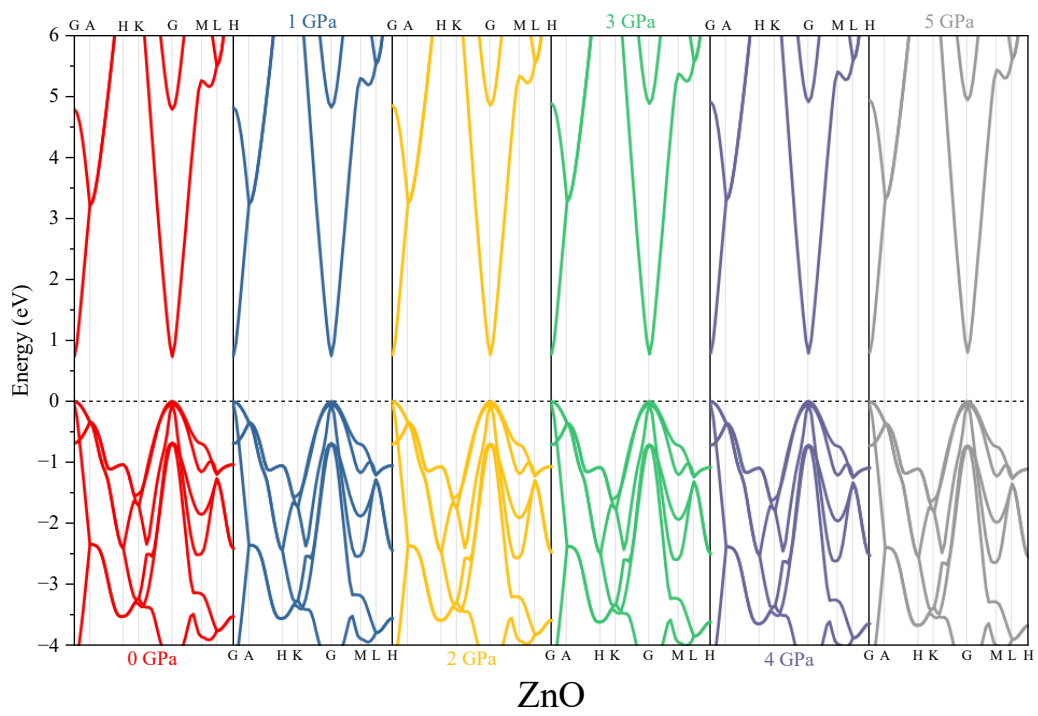


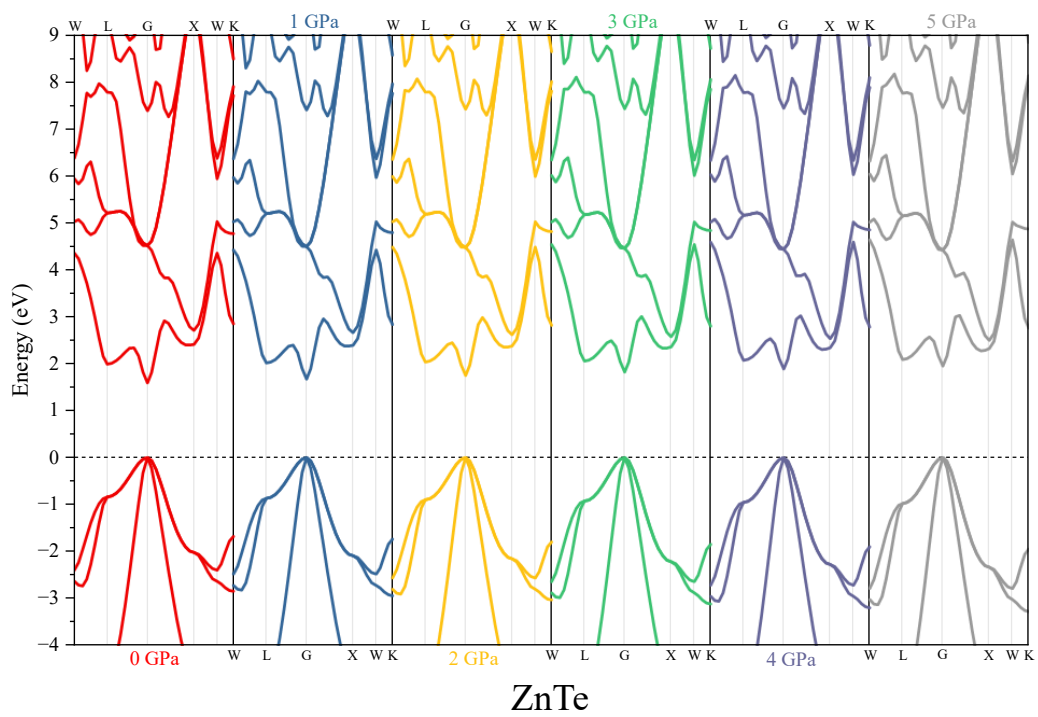
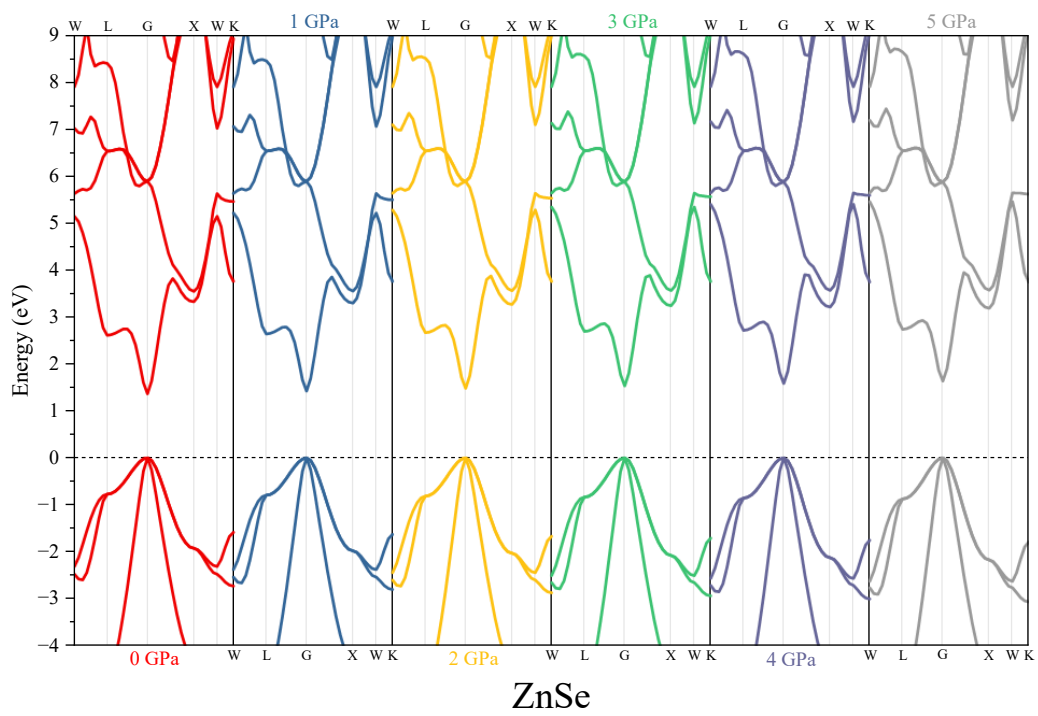


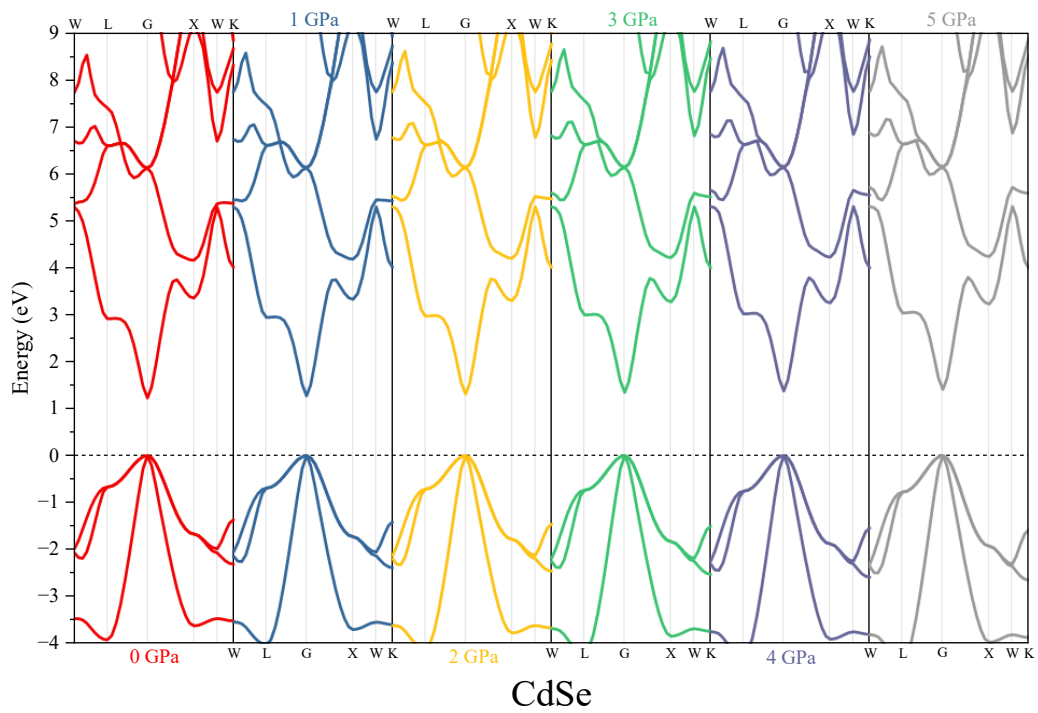
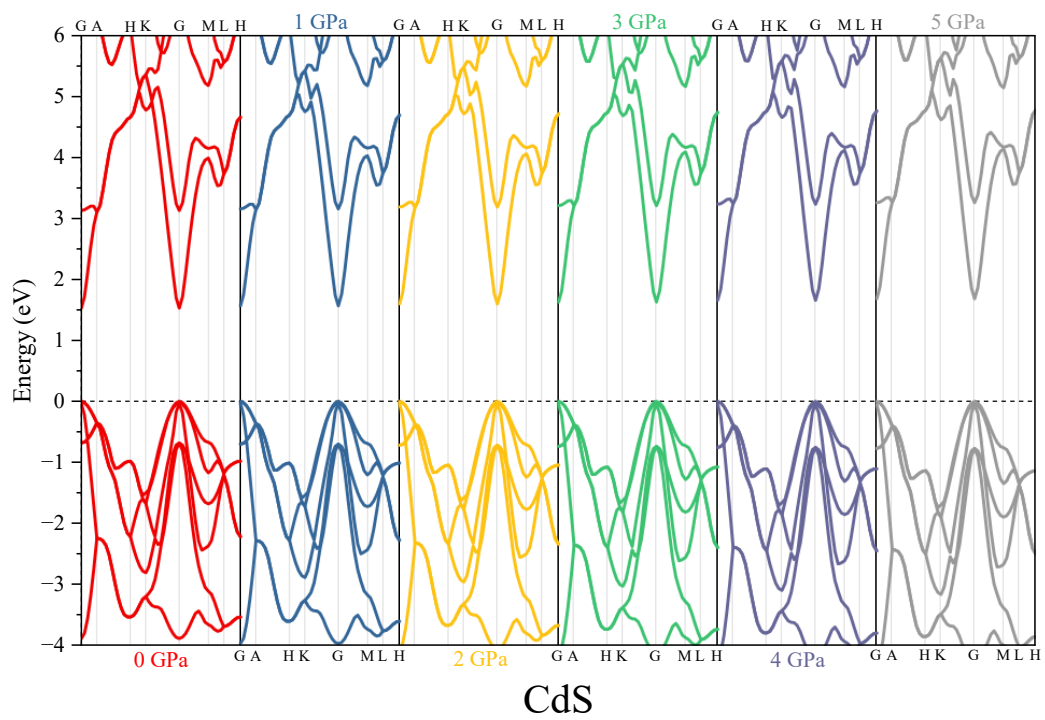
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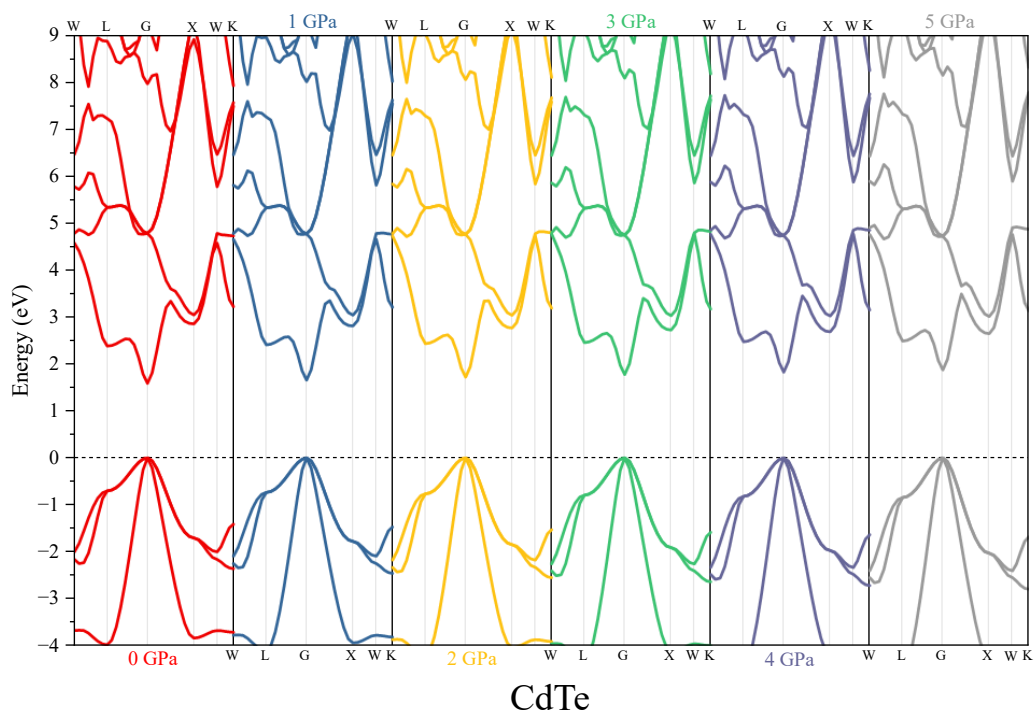


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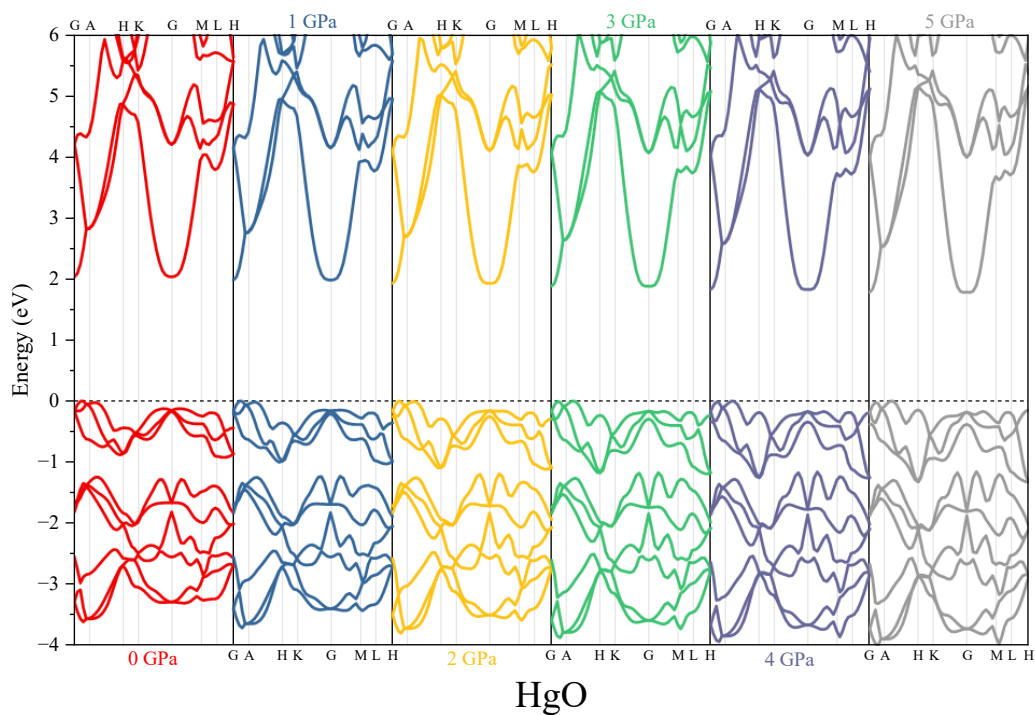




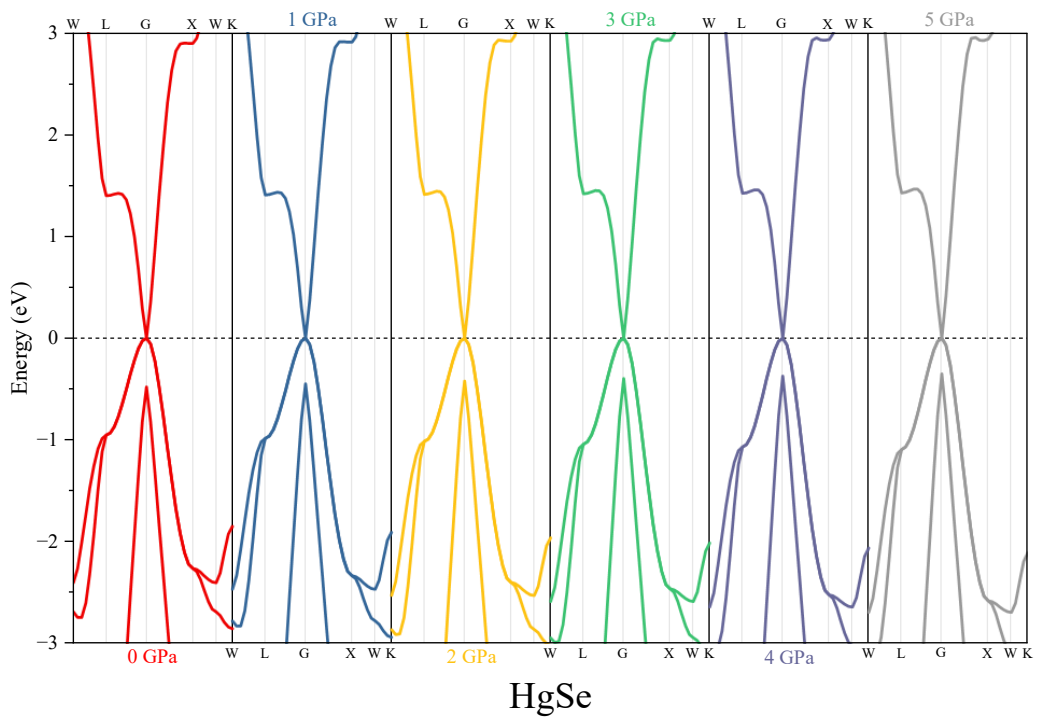
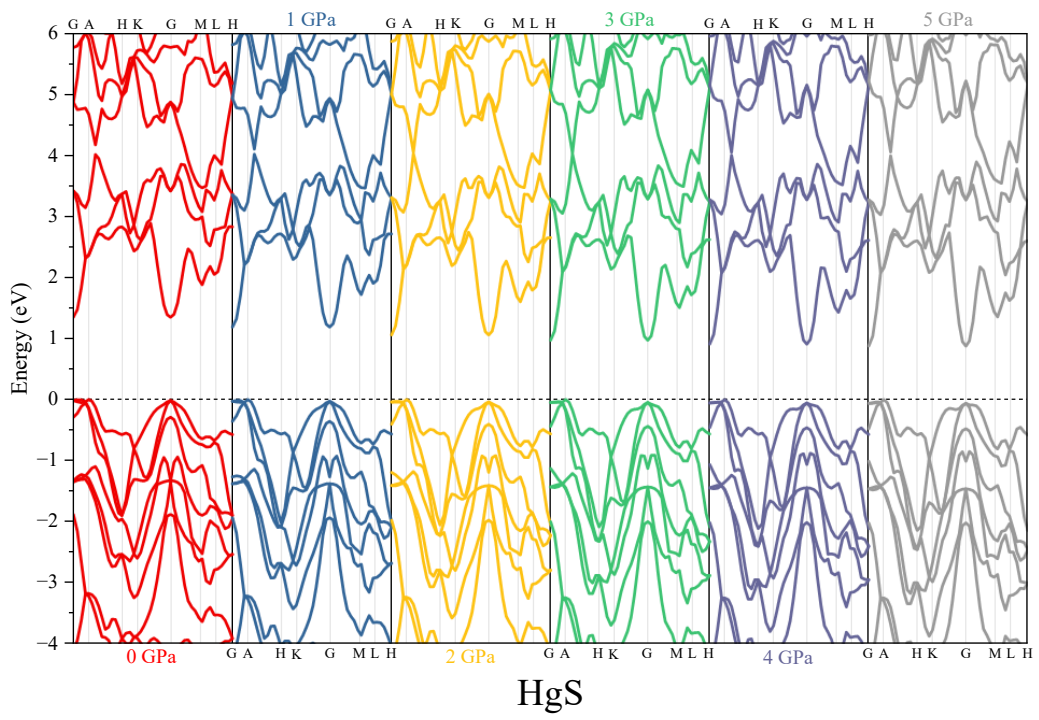


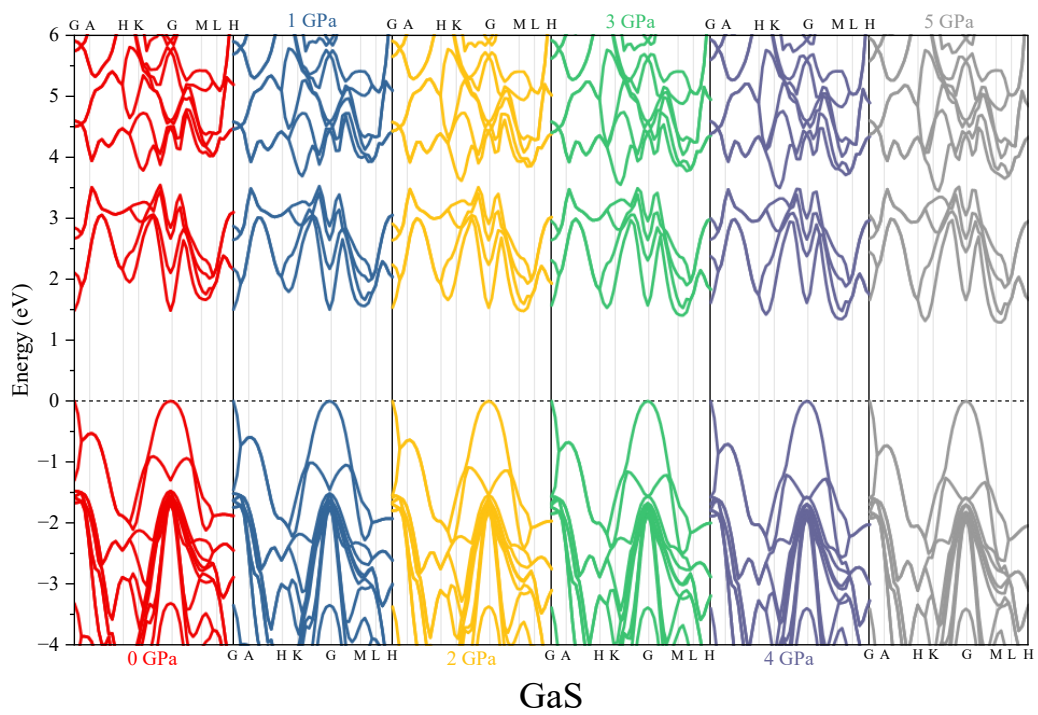
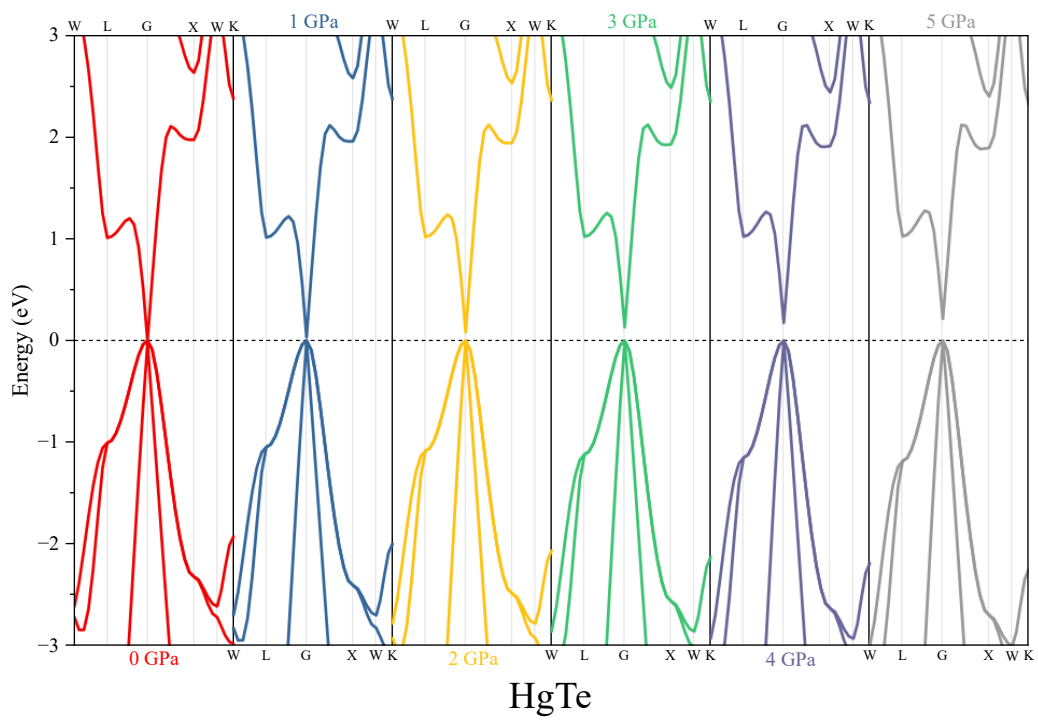


CdTe



HgO





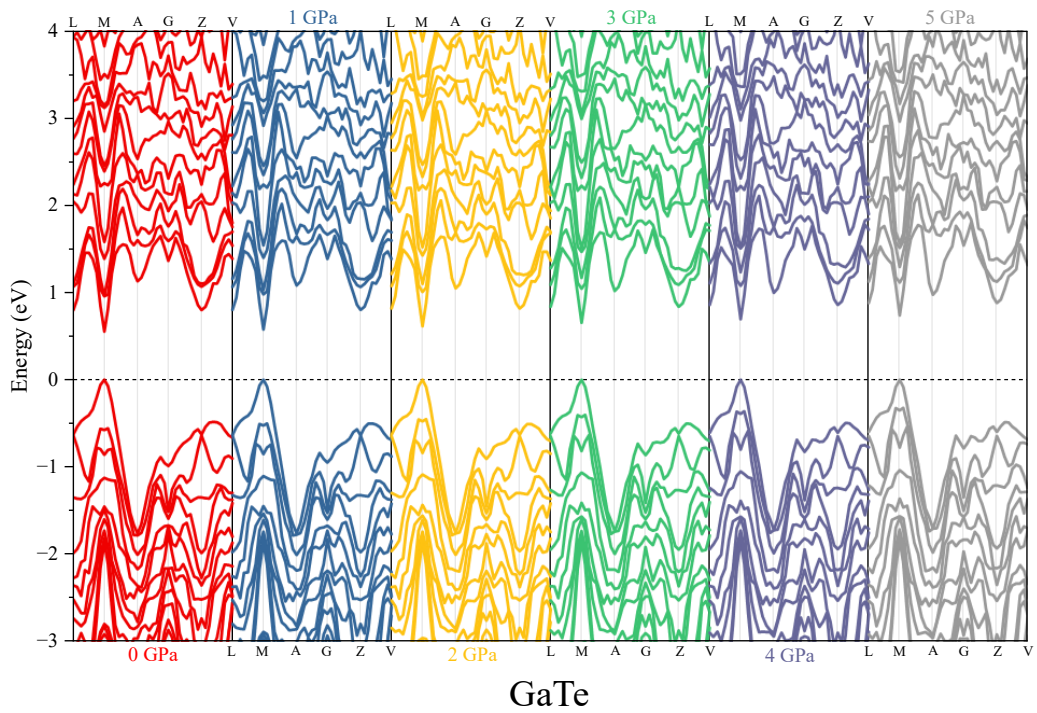
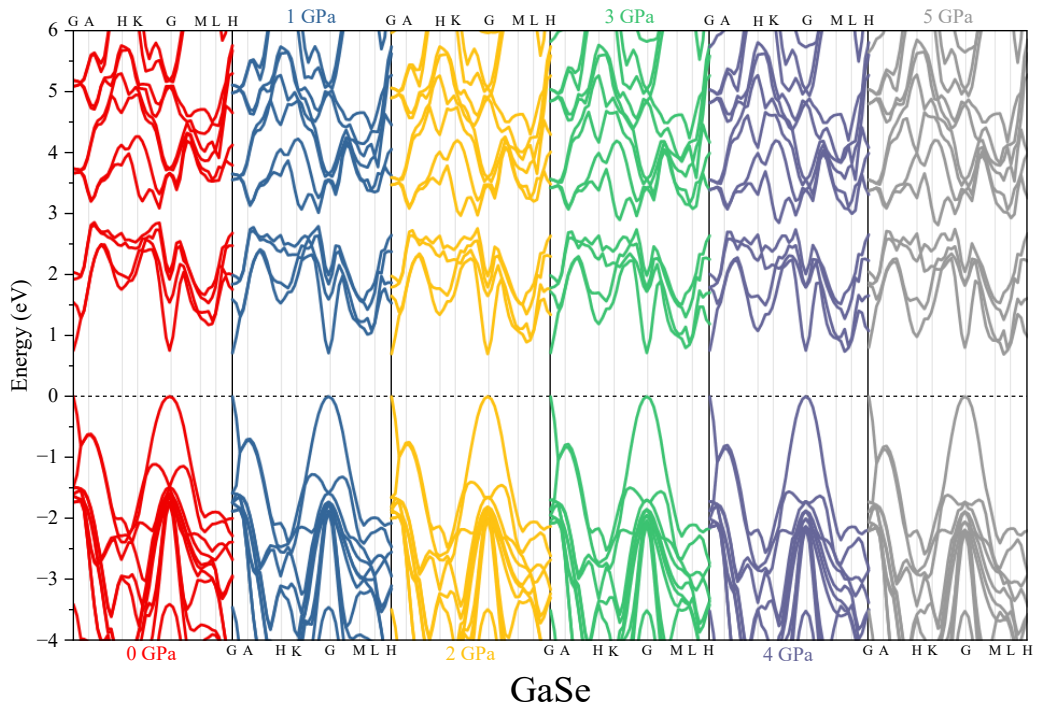


FIG. S2. The band structures under pressure from 0 to 5 GPa.

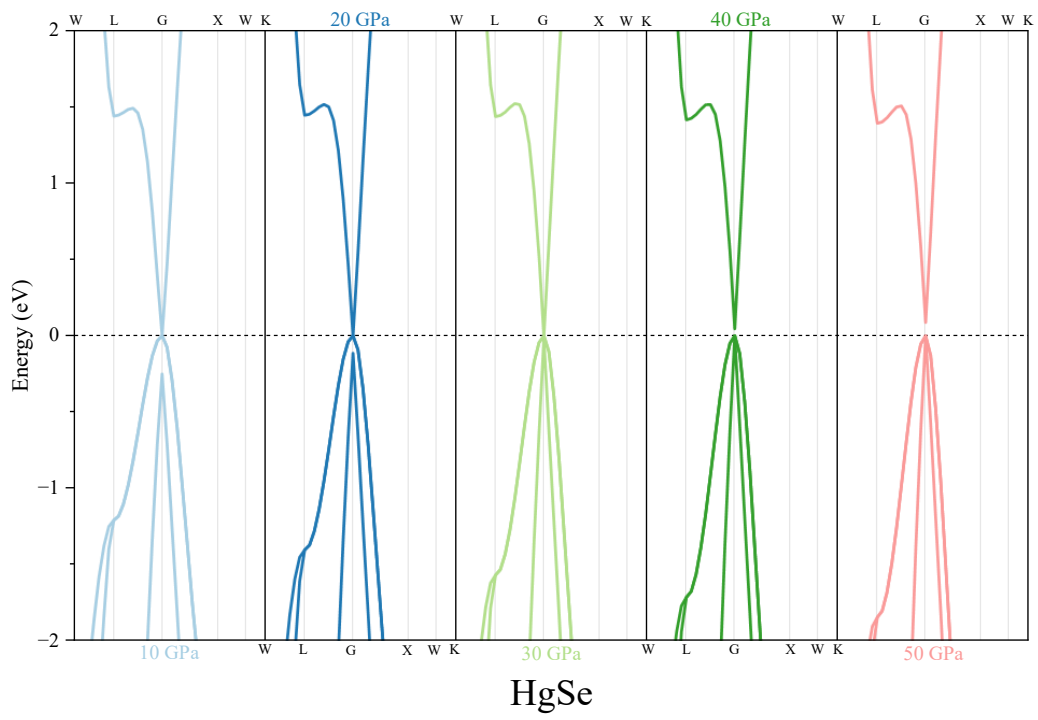


FIG. S3. The band structures of HgSe under pressure from 10 to 50 GPa.