

Supporting Information: 材料的非简谐性描述符研究

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表 S1 所选九种材料的体模量、热导率 (理论和实验)。

Table S1. Theoretical and experimental bulk moduli, thermal conductivities of nine selected materials.

晶体	体模量 B_L /GPa	晶格热导率理论值 $\kappa_{L(DFT)}(300\text{ K})/(\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1})$	热导率实验值 $\kappa_{L(expt.)}(300\text{ K})/(\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1})$
C	441.5	4022.4	2300.0
Si	97.6	110.0	148.0
Ge	69.3	35.4	67.0
Sn	40.2	5.3	60.0
GaAs	71.5	24.8	47.0
CdTe	37.3	3.9	7.5
NaCl	16.7	4.4	
γ -CsPbI ₃	12.6	0.08	
β -CsPbI ₃	14.3	0.11	

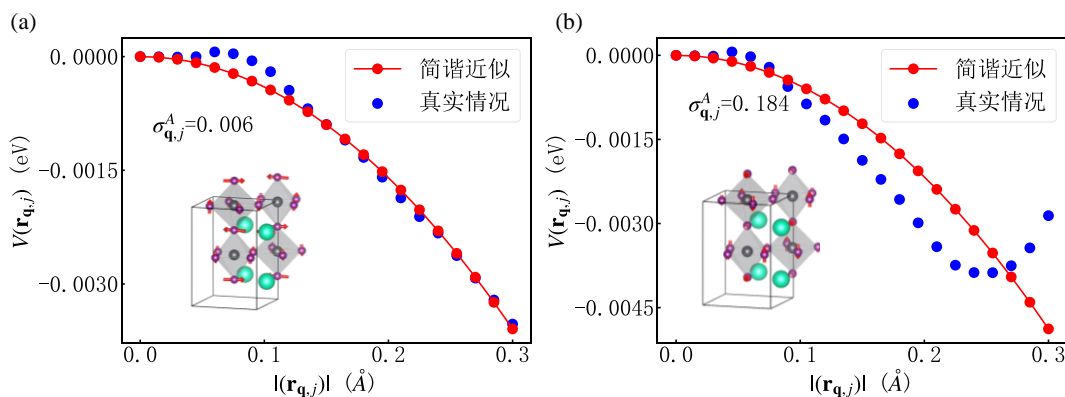


图 S1 β -CsPbI₃ 中两种不同的虚频声子振动模式的非简谐性示意图, 图中红色圆点表示完全简谐情况下声子振动对体系自由能的贡献 $V(\mathbf{r}_{q,j})$ 随着振动幅度 $|\mathbf{r}_{q,j}|$ 的变化趋势, 蓝色圆点则表示真实情况下其变化趋势

Fig.S1. Schematic diagrams of phonon anharmonicities of two types of imaginary phonon modes in β -CsPbI₃, with red dots representing change trend of contribution of phonon vibration to free energy of the system $V(\mathbf{r}_{q,j})$ with vibration amplitude $|\mathbf{r}_{q,j}|$ in harmonic approximation, and blue dots denoting change trend in the real case.

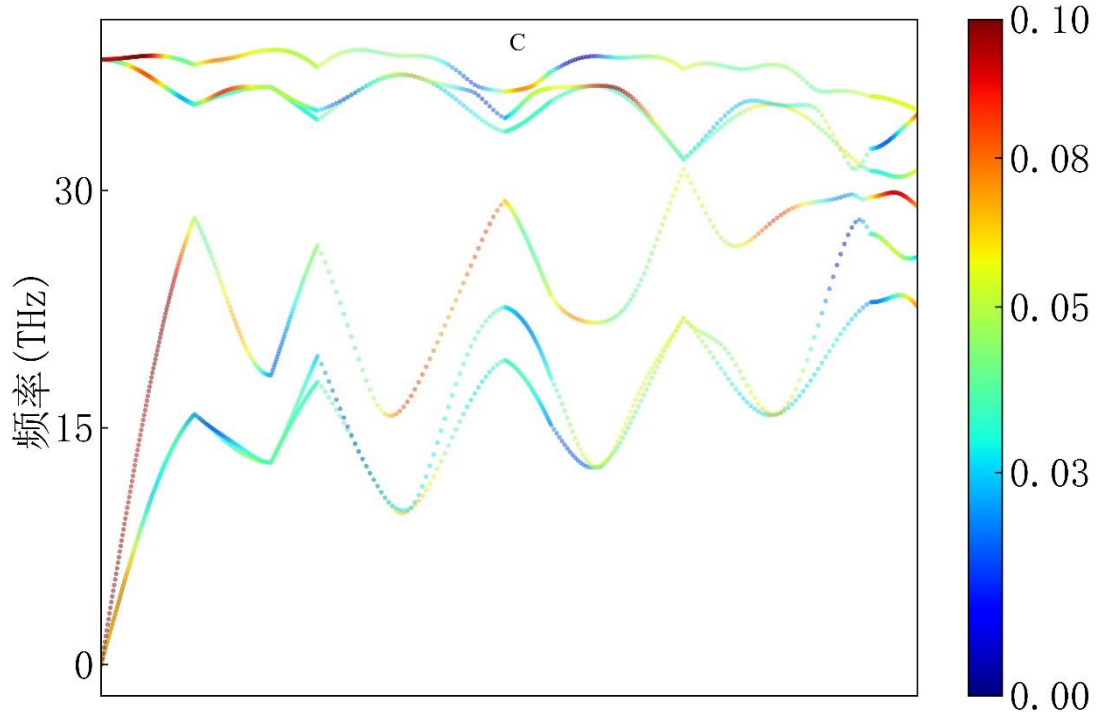


图 S2 C 晶体的声子谱，图中点的颜色值为对应声子模态的非简谐性描述符 $\sigma_{q,j}^A$

Fig. S2. Phonon spectra of C, with color value of point representing anharmonic descriptor $\sigma_{q,j}^A$ of corresponding phonon mode.

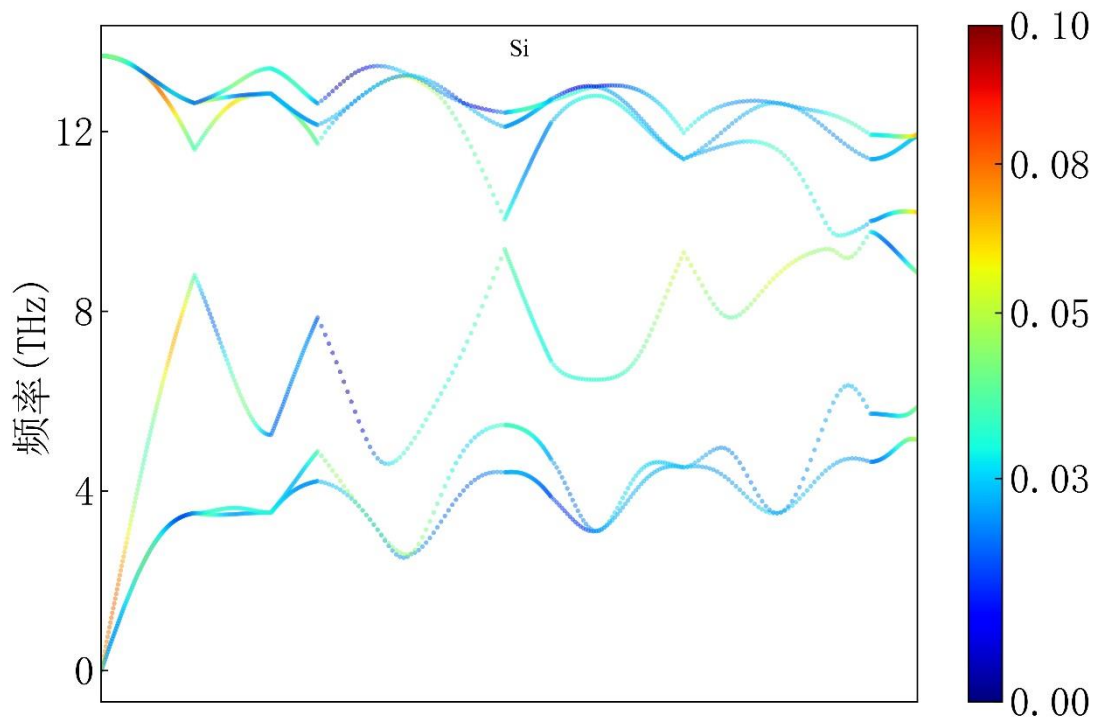


图 S3 Si 晶体的声子谱，图中点的颜色值为对应声子模态的非简谐性描述符 $\sigma_{q,j}^A$

Fig. S3. Phonon spectra of Si, with color value of point denoting anharmonic descriptor $\sigma_{q,j}^A$ of corresponding phonon mode.

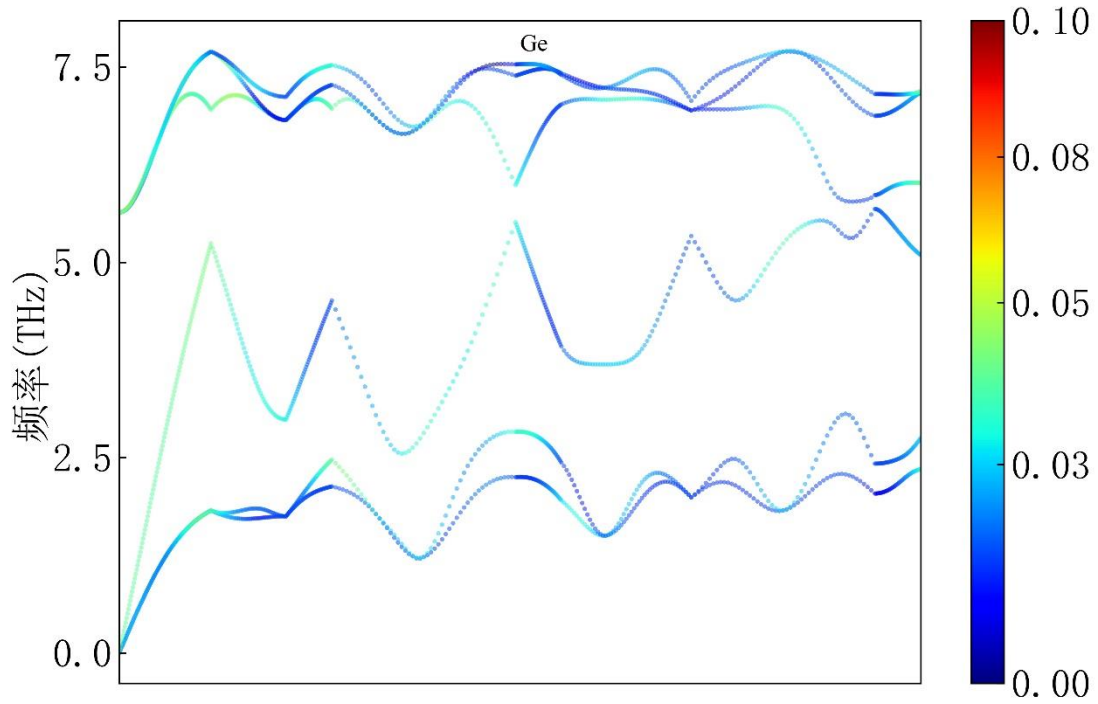


图 S4 Ge 晶体的声子谱，图中点的颜色值为对应声子模式的非简谐性描述符 $\sigma_{q,j}^A$

Fig. S4. Phonon spectra of Ge, with color value of point indicating anharmonic descriptor $\sigma_{q,j}^A$ of corresponding phonon mode.

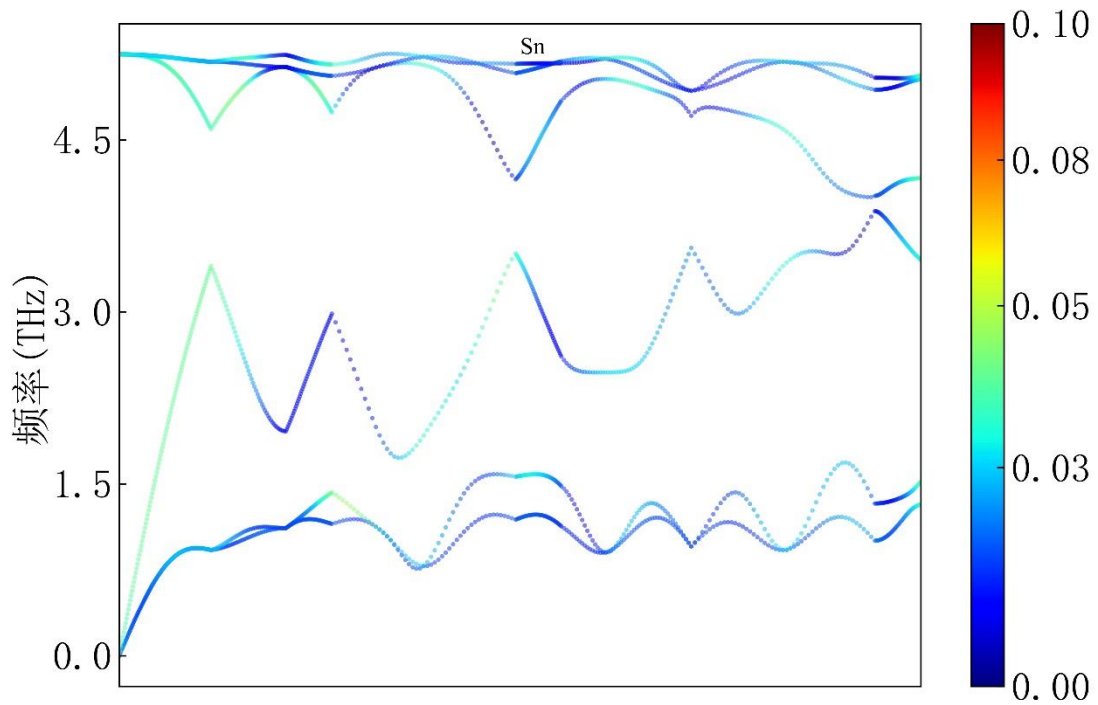


图 S5 Sn 晶体的声子谱，图中点的颜色值为对应声子模式的非简谐性描述符 $\sigma_{q,j}^A$

Fig. S5. Phonon spectra of Sn, with color value of point representing anharmonic descriptor $\sigma_{q,j}^A$ of corresponding phonon mode.

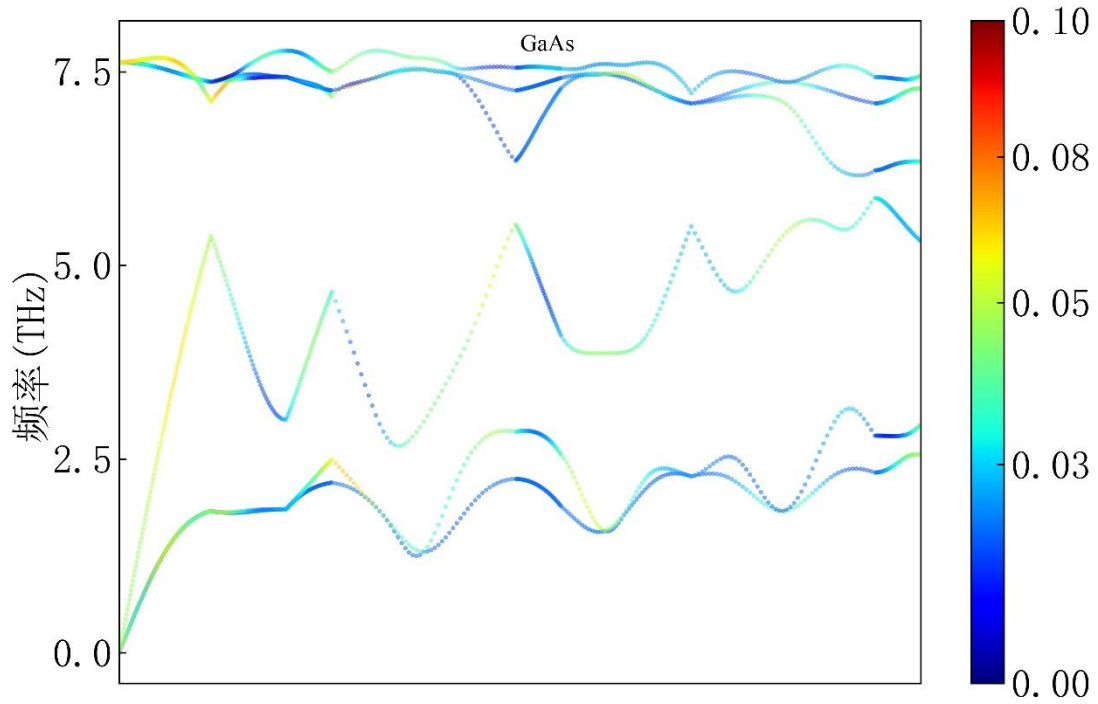


图 S6 GaAs 晶体的声子谱，图中点的颜色值为对应声子模式的非简谐性描述符 $\sigma_{q,j}^A$

Fig. S6. Phonon spectra of GaAs, with color value of point referring to anharmonic descriptor $\sigma_{q,j}^A$ of corresponding phonon mode.

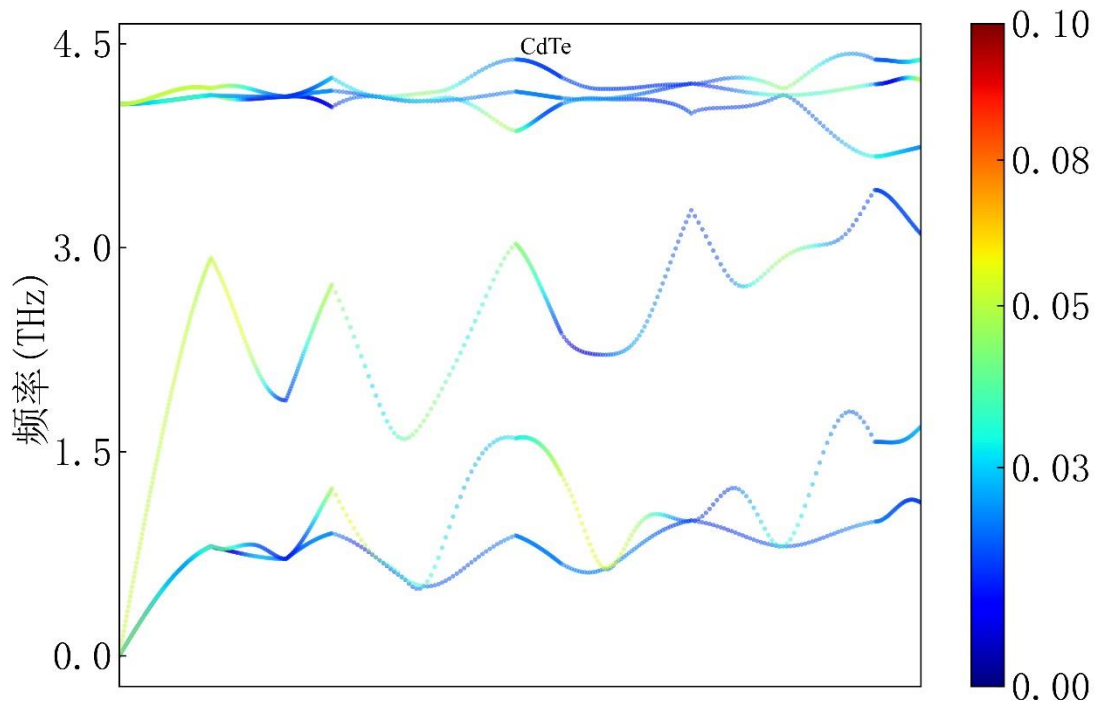


图 S7 CdTe 晶体的声子谱，图中点的颜色值为对应声子模式的非简谐性描述符 $\sigma_{q,j}^A$

Fig. S7. Phonon spectra of CdTe, with color value of point in graph representing anharmonic descriptor $\sigma_{q,j}^A$ of corresponding phonon mode.

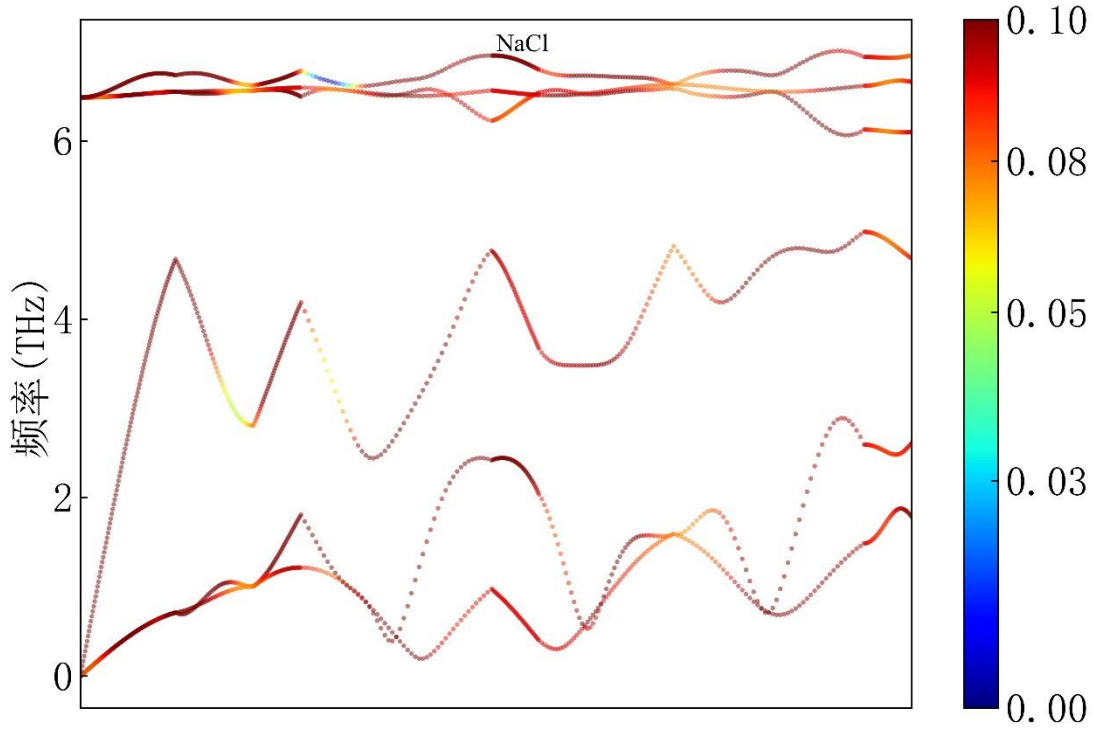


图 S8 NaCl 晶体的声子谱，图中点的颜色值为对应声子模式的非简谐性描述符 $\sigma_{q,j}^A$

Fig. S8. Phonon spectra of NaCl, with color value of point denoting anharmonic descriptor $\sigma_{q,j}^A$ of corresponding phonon mode.

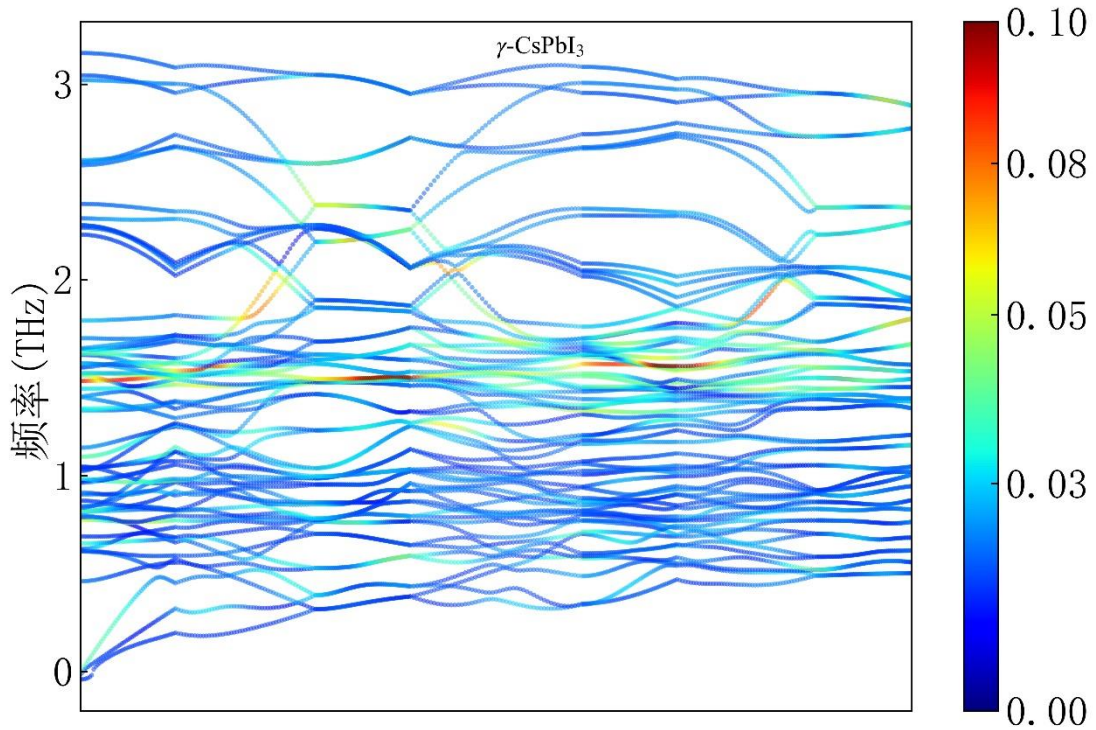


图 S9 γ -CsPbI₃ 晶体的声子谱，图中点的颜色值为对应声子模式的非简谐性描述符 $\sigma_{q,j}^A$

Fig. S9. Phonon spectra of γ -CsPbI₃, with color value of point referring to anharmonic descriptor $\sigma_{q,j}^A$ of corresponding phonon mode.

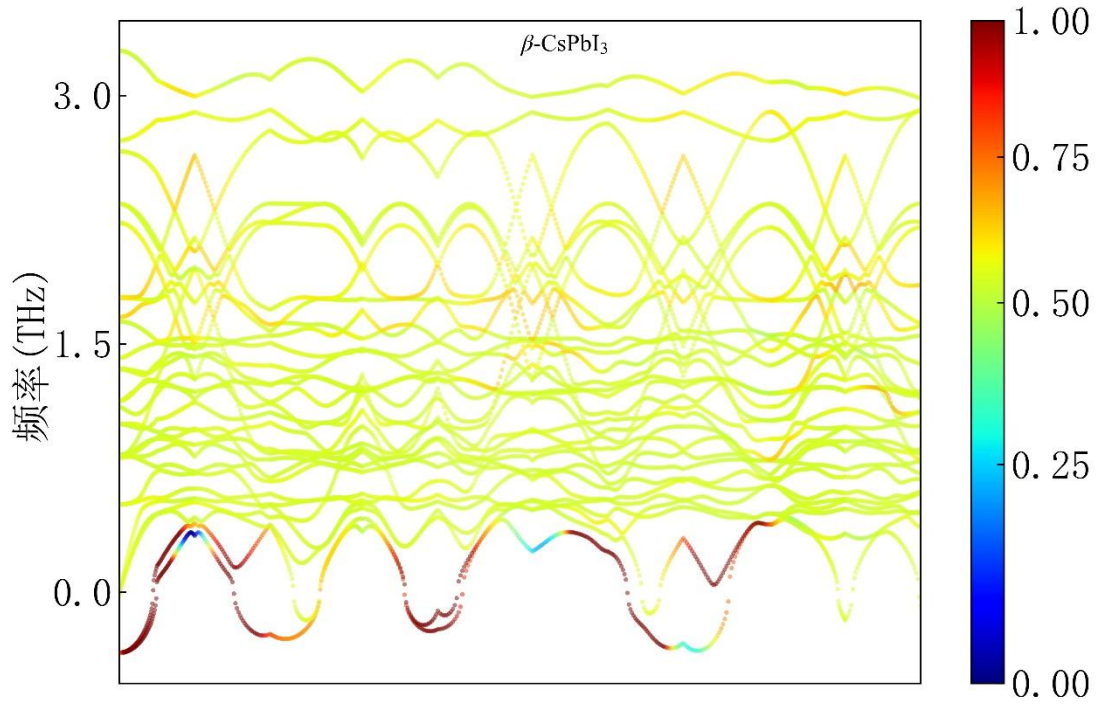


图 S10 β -CsPbI₃ 晶体的声子谱，图中点的颜色值为对应声子模式的非简谐性描述符 $\sigma_{q,j}^A$

Fig. S10. Phonon spectra of β -CsPbI₃, with color value of point representing anharmonic descriptor $\sigma_{q,j}^A$ of corresponding phonon mode.