

Pressure induced excellent thermoelectric behavior in skutterudites CoSb_3 and IrSb_3

Xiuxian Yang,¹ Zhenhong Dai,^{1,*} Yinchang Zhao,^{1,†}

Wenchao Niu,¹ Jianye Liu,¹ and Sheng Meng^{2,3,‡}

¹*Department of Physics, Yantai University,
Yantai 264005, People's Republic of China*

²*Beijing National Laboratory for Condensed Matter Physics and Institute of Physics,
Chinese Academy of Sciences, Beijing,
100190, People's Republic of China*

³*Collaborative Innovation Center of Quantum Matter,
Beijing 100084, People's Republic of China*

(Dated: October 15, 2018)

PACS numbers: 65.40.-b, 66.70.-f, 63.20.-e, 72.20.-i

A. S1.

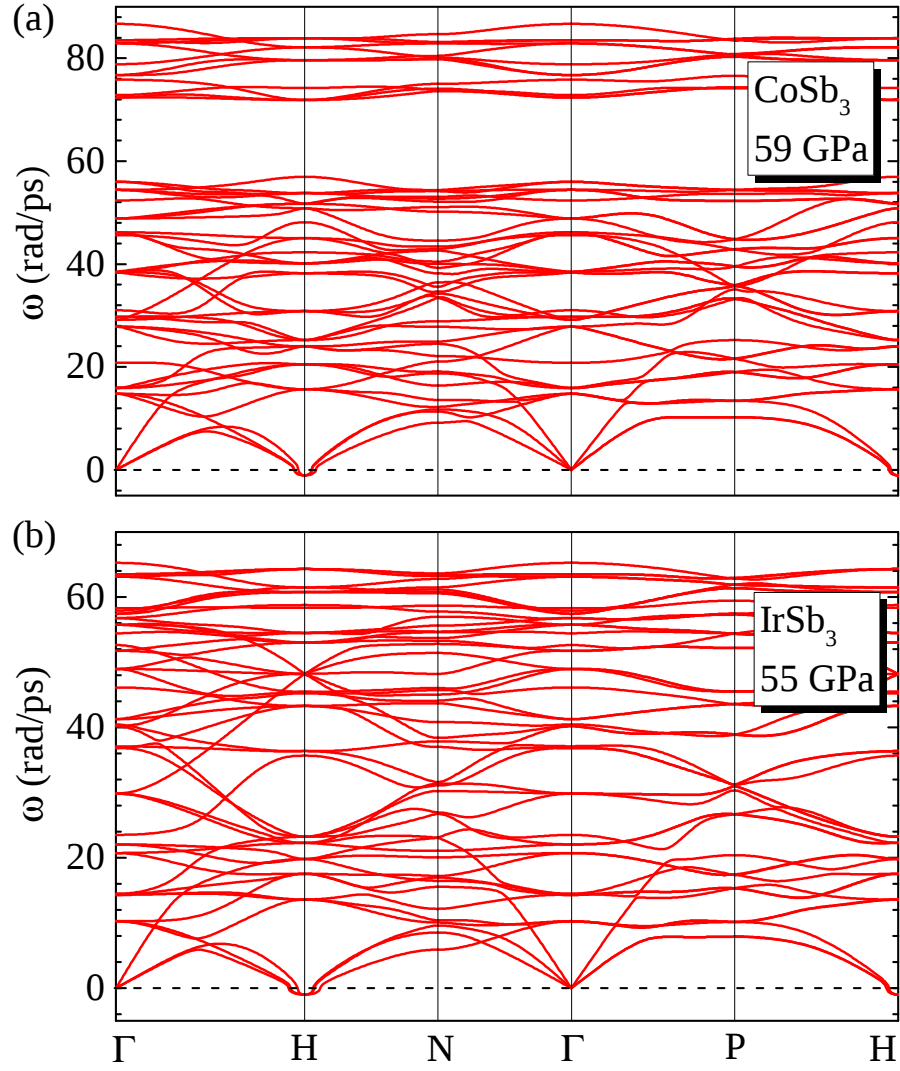


FIG. S1. (Color online). Phonon dispersion relations of CoSb_3 (a) at 59 GPa and IrSb_3 (b) at 55 GPa along the high symmetry point within the first Brillouin zone (BZ), respectively.

TABLE I. Pressure-Volume Relation for IrSb₃ is from the experimental data[40].

P	a	V
GPa	Å	Å ³
1.9	9.211	781.52
4.2	9.1867	775.31
4.7	9.1491	765.84
6.3	9.1350	762.31
9.5	9.0706	746.29
14.3	8.9956	727.93
15.3	8.9771	723.44
20.8	8.8887	702.29
23.9	8.8649	696.65
26.0	8.8261	687.55
33.8	8.7391	667.43
42.2	8.6731	652.40

B. S2.

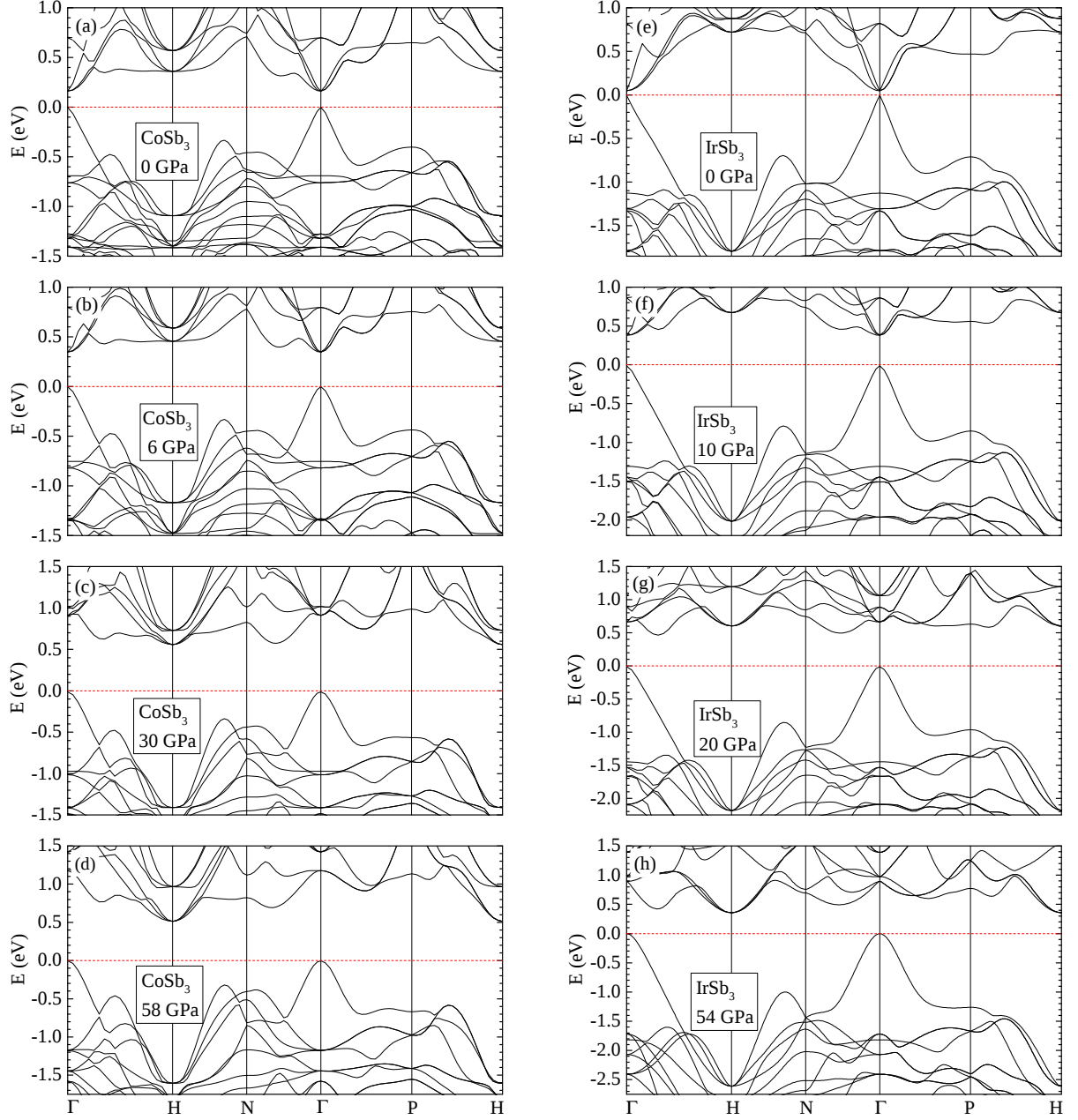


FIG. S2. (Color online). Electron bands of CoSb_3 (IrSb_3) at 0 GPa, 6 (10) GPa, 30 (20) GPa, and 58 (54) GPa along the high symmetry point within the first Brillouin zone (BZ), respectively.

C. S3.

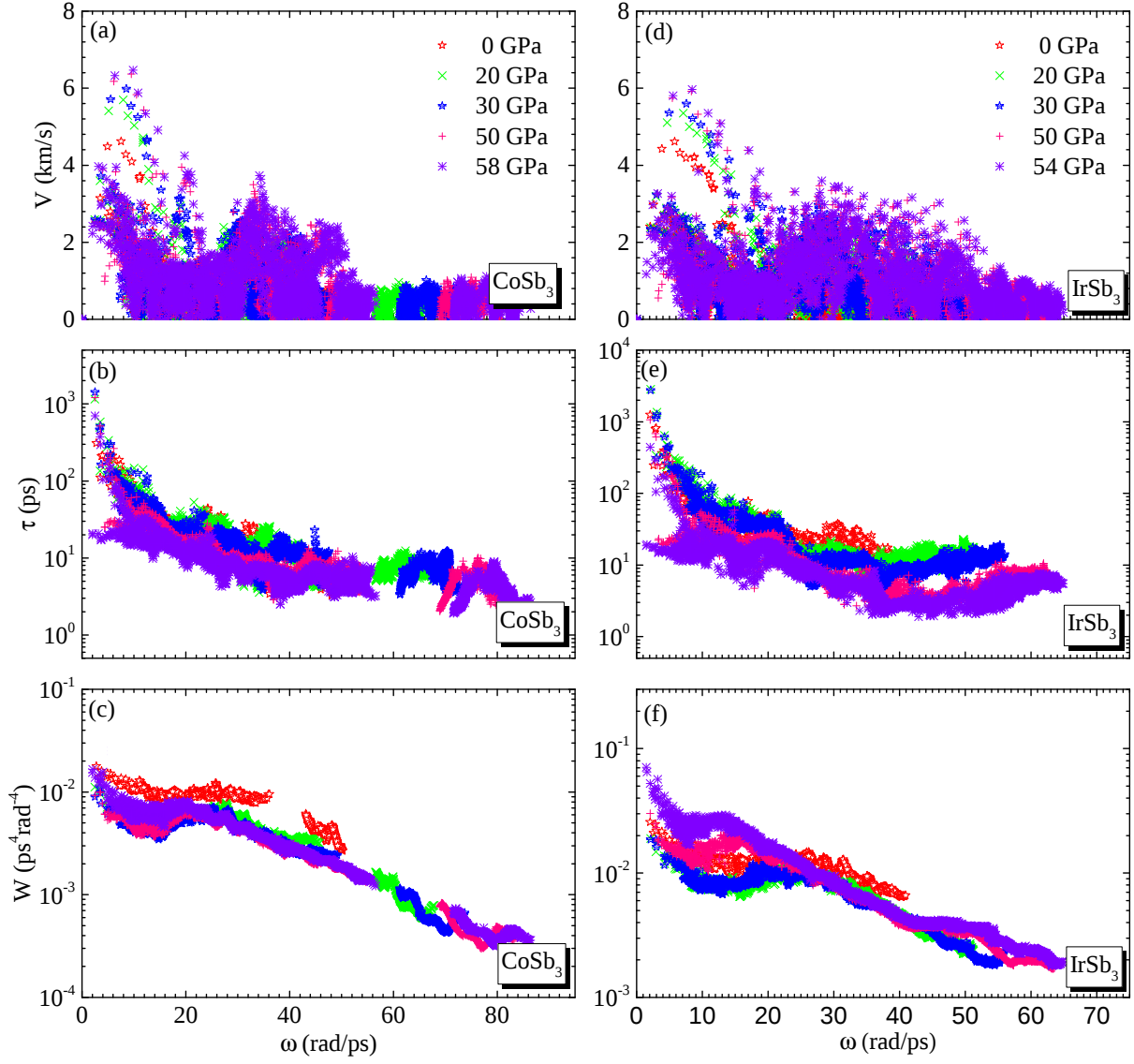


FIG. S3. (Color online). Frequency dependent phonon group velocities (a)(d), the anharmonic relaxation times τ (b)(e), and the weight phase space W (c)(f) within the first Brillouin zone (BZ) for CoSb₃ and IrSb₃ at 300 K, respectively.

D. S4.

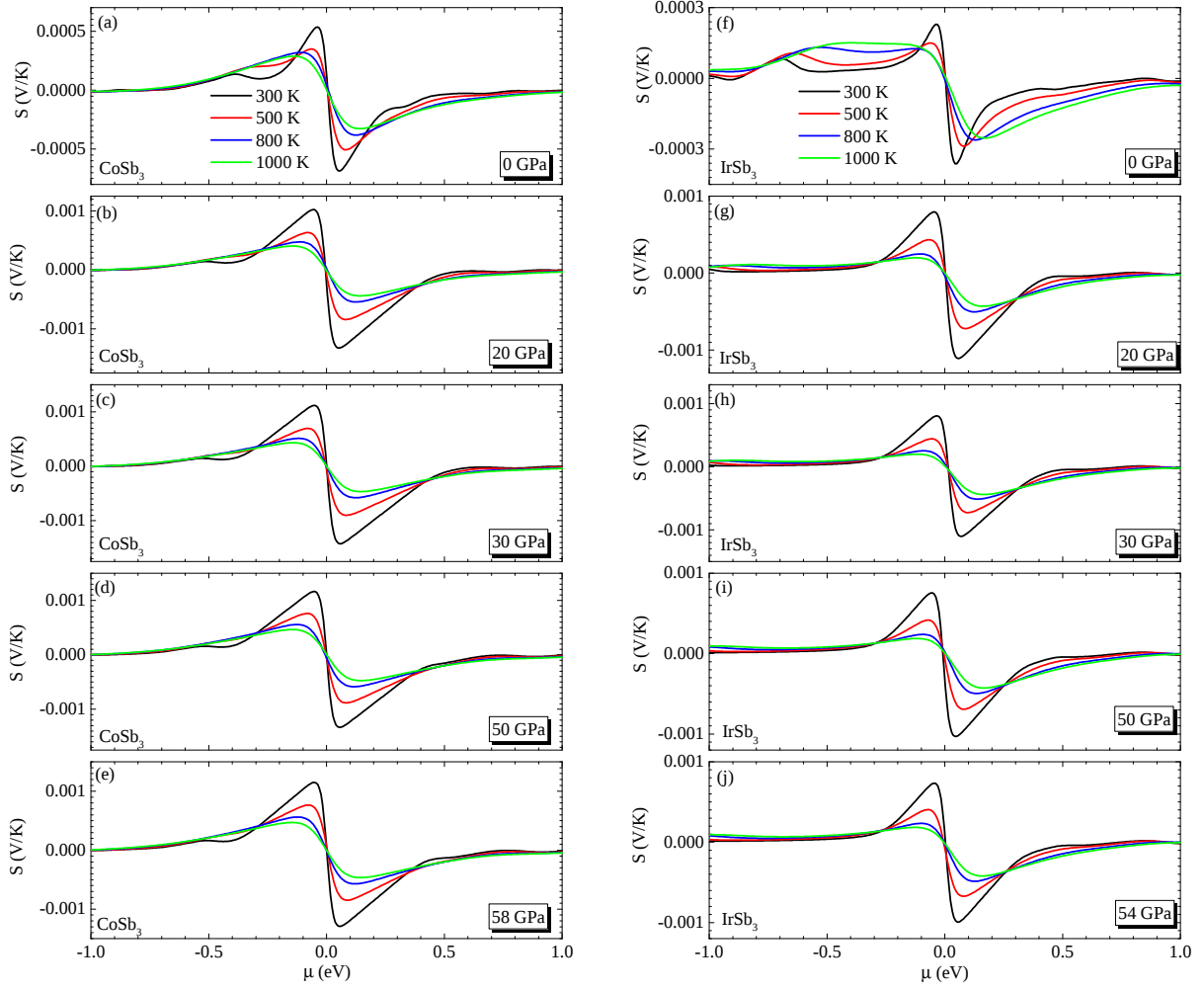


FIG. S4. (Color online). The S of different pressure (0, 20, 30, 50, 58, 54 GPa) at different temperature (300, 500, 800, 1000K) for these materials.

E. S5.

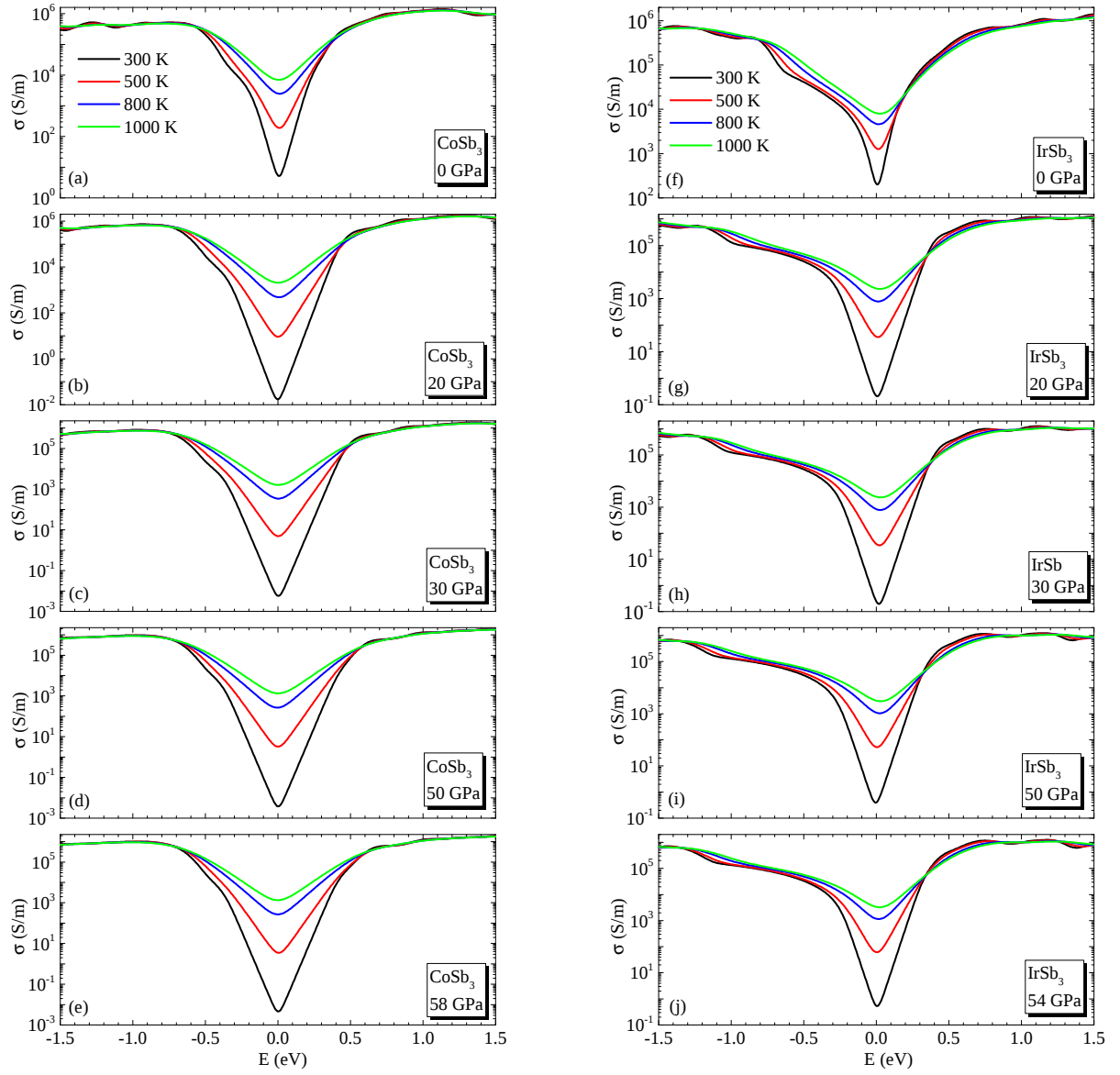


FIG. S5. (Color online). The electrical conductivity σ under different pressures.

F. S6.

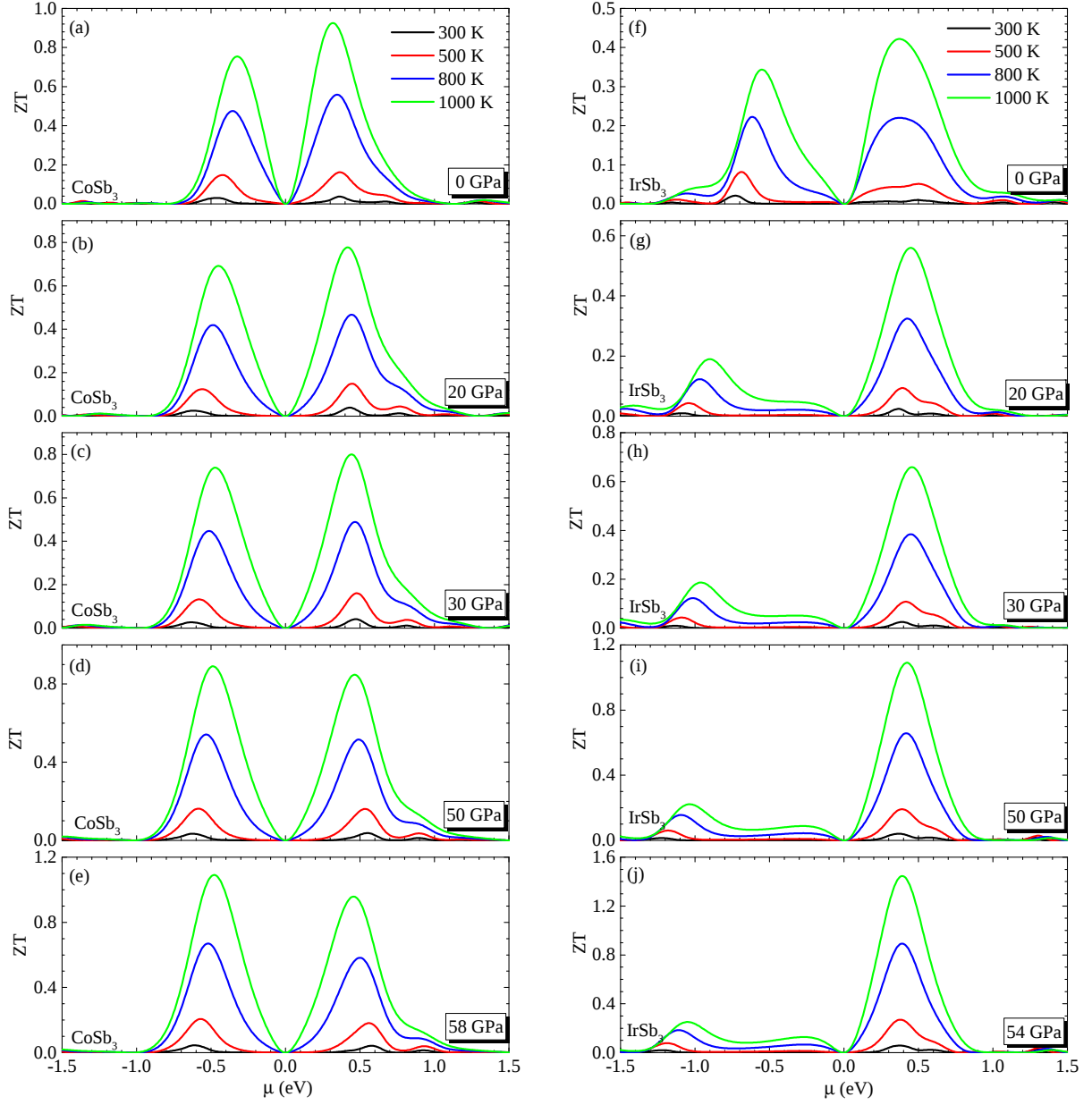


FIG. S6. The figure of merit ZT of CoSb_3 and IrSb_3 under different pressures. The black, red, blue, and green lines express 300K, 500K, 800K and 1000K, respectively.

G. S7.

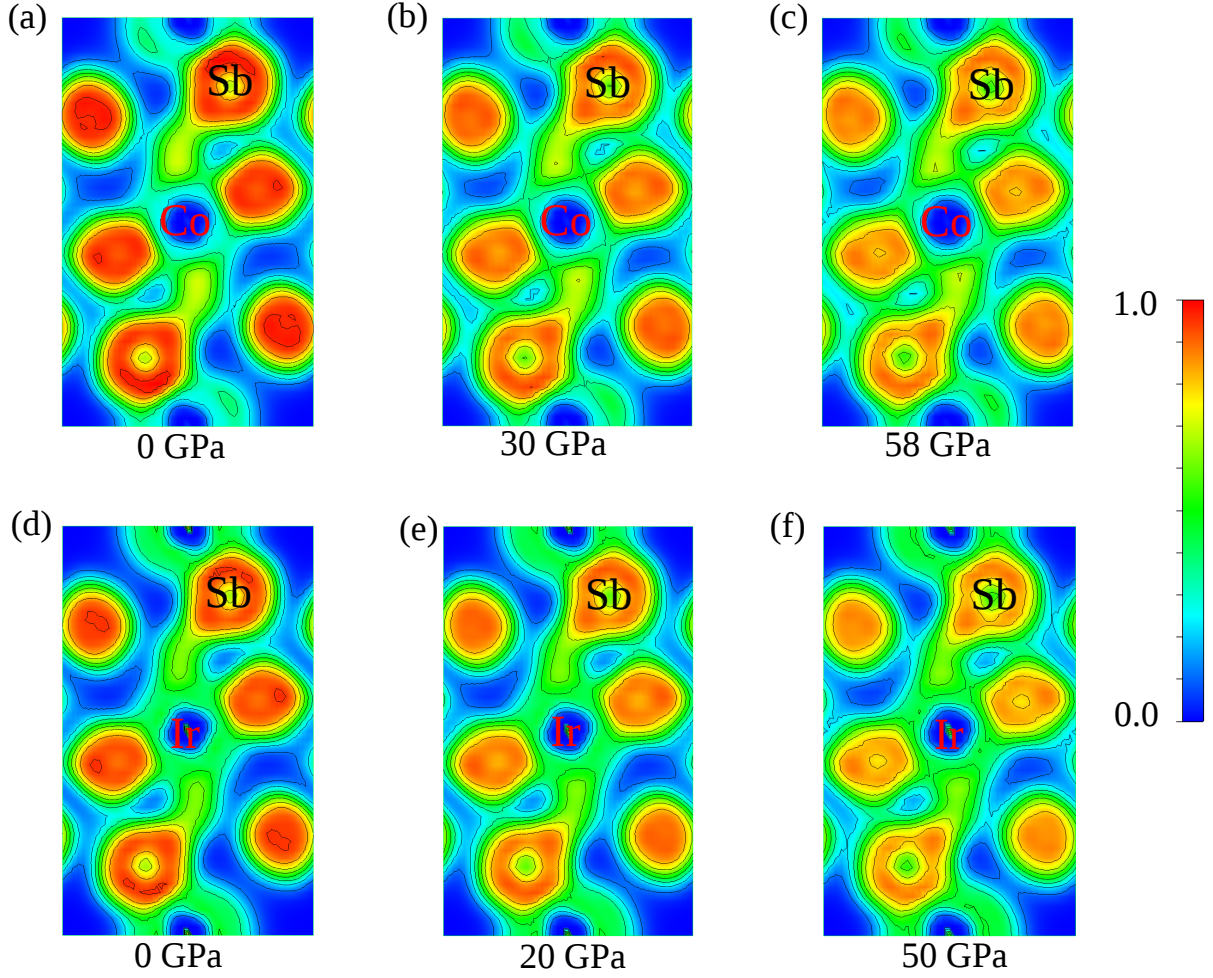


FIG. S7. (Color online). Electron localization function (ELF), which measures spatial localization of electrons plotted in the [110] plane at different pressure. Simply, we chose 0GPa (initial pressure), 30GPa (intermediate pressure), 58GPa (critical pressure) for CoSb₃ (a-c) and 0GPa (initial pressure), 20GPa (intermediate pressure), 54GPa (critical pressure) for IrSb₃ (d-f).

* zhdai@ytu.edu.cn

† y.zhao@ytu.edu.cn

‡ smeng@iphy.ac.cn