Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Influence of the stacking sequence on layered-chalcogenides properties: First principle investigation of $Pb_2Bi_2Te_5$

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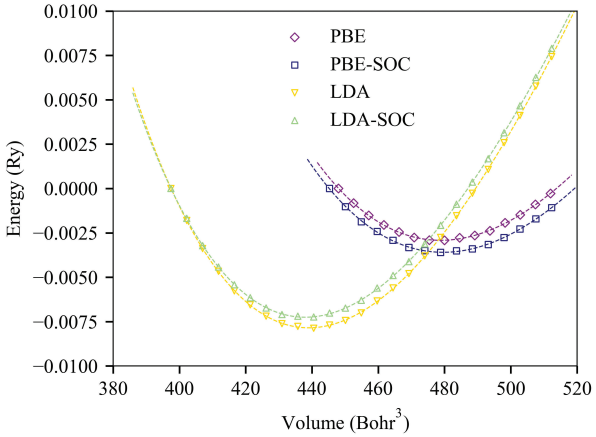

Figure S1 Relative energy versus cell volume for PbTe.

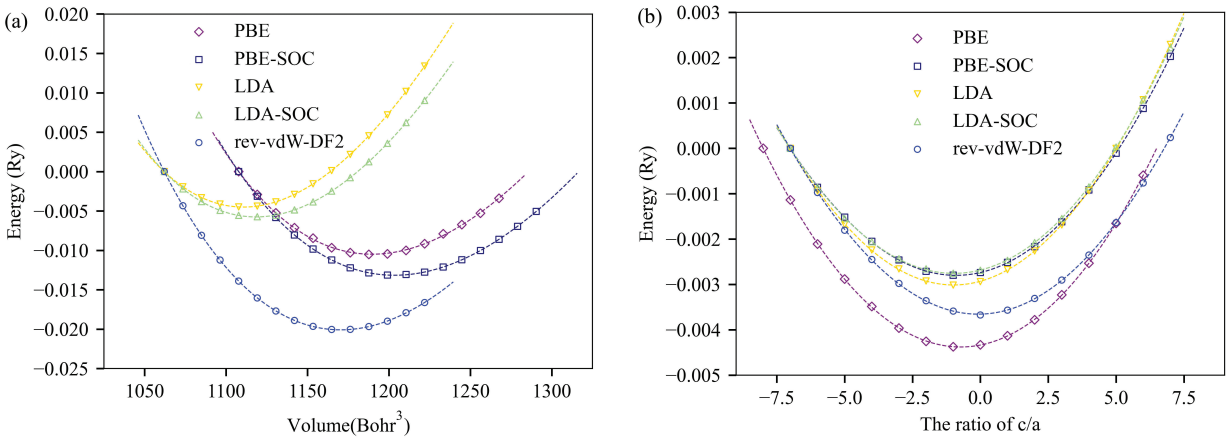

Figure S2 Relative energy versus cell volume (a) and a/c ratio (b) for Bi_2Te_3.

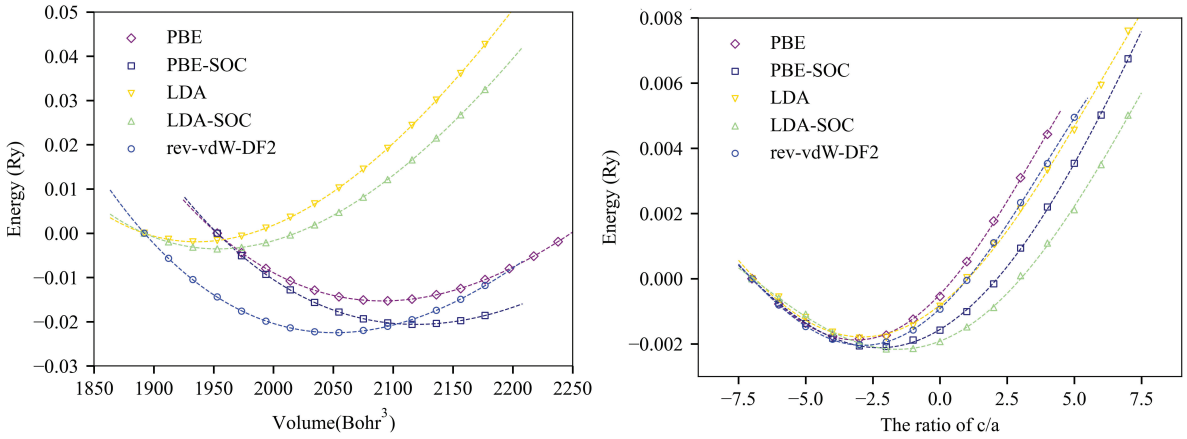

Figure S3 Relative energy versus cell volume (a) and a/c ratio (b) for $Pb_2Bi_2Te_5$ with stacking A.

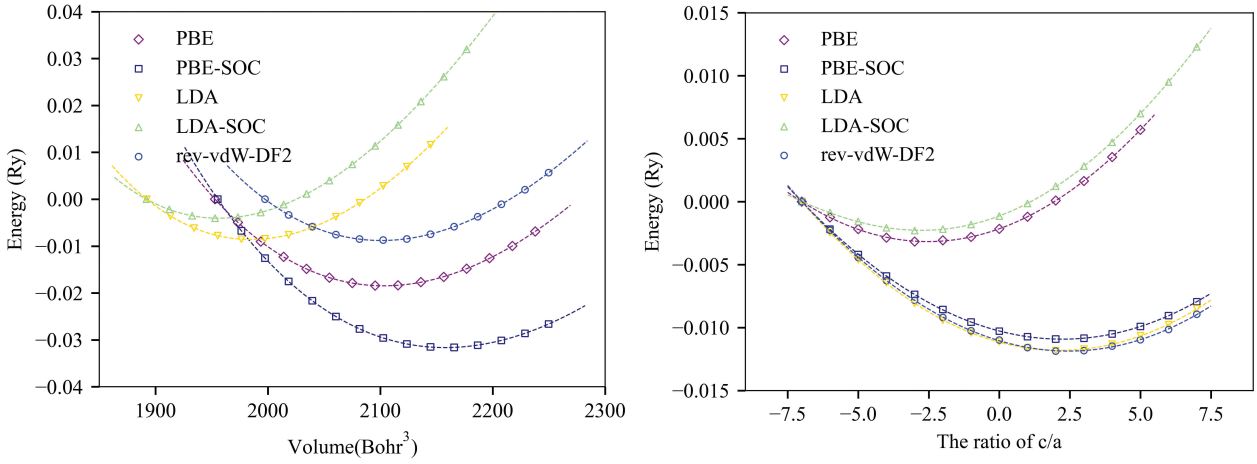

Figure S4 Relative energy versus cell volume (a) and a/c ratio (b) for $Pb_2Bi_2Te_5$ with stacking B.

Table S1 Topological properties of PbTe and Bi_2Te_3 corresponding to the BCPs in Figure S8a,b; r1 is the distance between BCP and Bi; r2 is the distance between BCP and Te; r1 and r2 are in unit of pm; the angle is between BCPs and their two ends; ρ and $\nabla^2\rho$ are the electron charge density and its Laplacian at the BCPs in unit of 10^{-2}e/bohr^3 and 10^{-2}e/bohr^5; G, V and H represent the kinetic, potential and total energy densities at the BCPs in unit of 10^{-2}a.u./bohr^3.

BCP	r1	r2	r1/r2	angle	ρ	$\nabla^2\rho$	G	V	H	$\lvert V\rvert/G$	H/ρ
PbTe-b	158.2	170.4	0.9286	180.00	2.672	3.111	1.20	-1.63	-0.43	1.35	-1.60
Bi2Te3-b1	157.5	165.3	0.9526	179.84	3.095	3.168	1.40	-2.02	-0.61	1.44	-1.98
Bi2Te3-b2	149.2	156.7	0.9526	179.64	4.267	2.710	1.95	-3.22	-1.27	1.65	-2.98
Bi2Te3-b3	178.0	178.0	1.0000	180.00	1.379	2.075	0.75	-0.88	-0.13	1.18	-0.75

Table S2 Electron charge density ($10^2\rho$ in e/bohr^3) at the bond critical points along the slab for stacking-A-sequence structures with 9 (S1-1) and 21 (S1-2) layers, for stacking-B-sequence structures with 9 (S2-1) and 21 (S2-2) layers and stacking-B-sequence structures with the Bi atom replaced by a Pb one with 9 (S3-1) and 21 (S3-2) layers. The critical point numbered 1 corresponds to the Te-Te bond across the gap between the slabs.

	1	2	3	4	5	6	7	8	9	10	11
S1-1	1.77	4.15	1.99	4.02	3.06						
S2-1	1.38	4.08	2.83	2.90	2.86						
S3-1	1.69	3.60	2.26	2.98	2.67						
S1-2	1.41	4.06	1.71	3.93	2.93	3.04	3.57	2.54	3.58	2.75	3.20
S2-2	1.04	3.94	2.69	2.75	2.70	2.74	2.73	2.74	2.73	2.74	2.74
S3-2	1.70	3.62	2.19	3.02	2.49	2.87	2.61	2.79	2.67	2.75	2.71

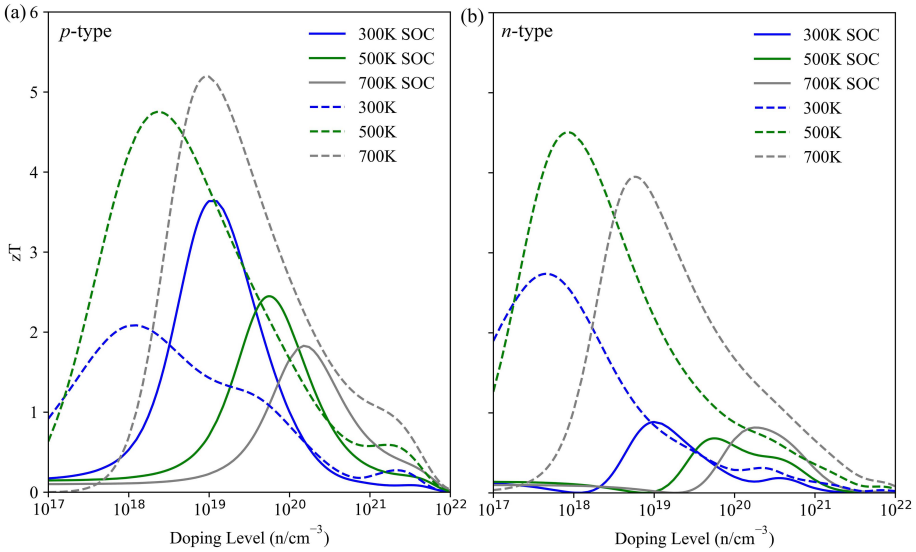

Figure S5 Calculated figure of merit zT of Pb2Bi2Te5 stacking A with *p*-type (a) and *n*-type (b). The solid and dash lines represent zT with and without SOC.

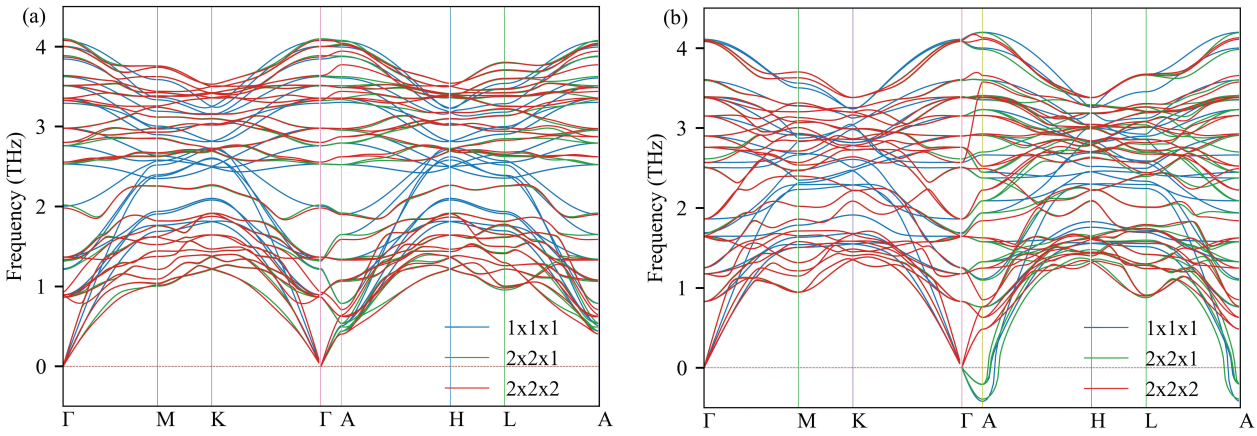

Figure S6 Phonon dispersion convergence of $Pb_2Bi_2Te_5$ stacking A (a) and stacking B (b) with 1×1×1, 2×2×1 and 2×2×2 supercell.

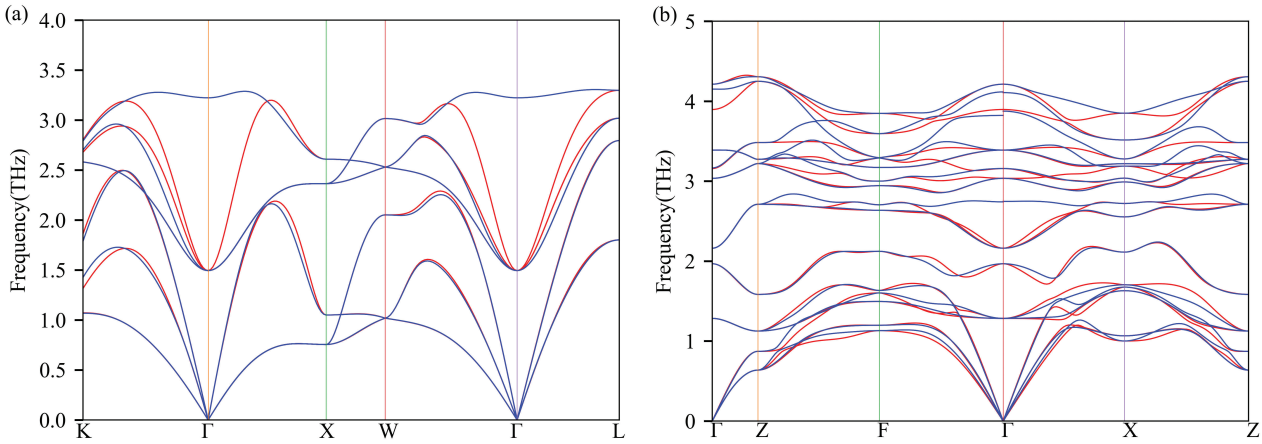

Figure S7 Phonon dispersion of PbTe (a) and Bi_2Te_3 (b) with (blue line) and without (red line) LO-TO splitting effect. Long-range electrostatic interactions are included by evaluating the dielectric tensor and Born effective charges using density functional perturbation theory.

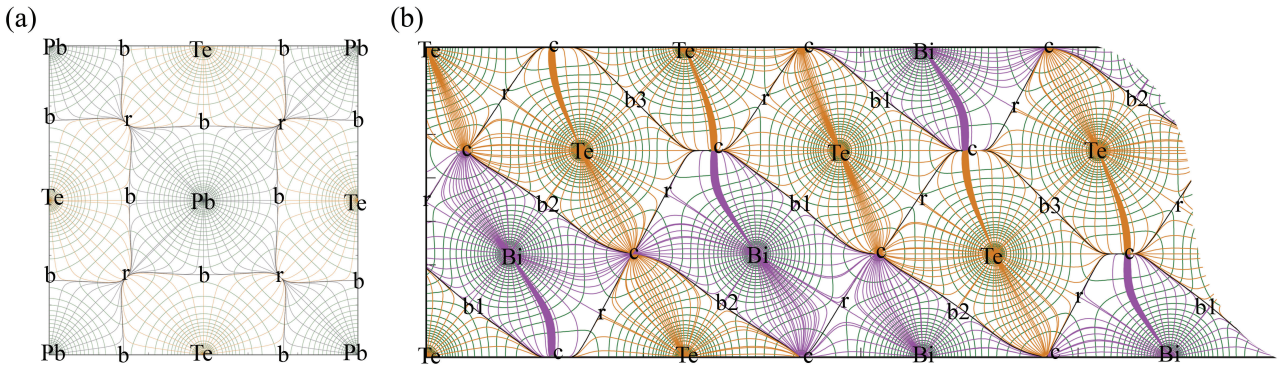

Figure S8 CPs and flux lines derived from $\nabla\rho(r)$ (light green lines) of PbTe (a) in (100)-plane and Bi_2Te_3 (b) in (110)-plane.