

Supplementary Information

First-principles study of the effect of multi-Dirac phonons on the thermoelectric properties in Janus BiSbC₃ monolayer

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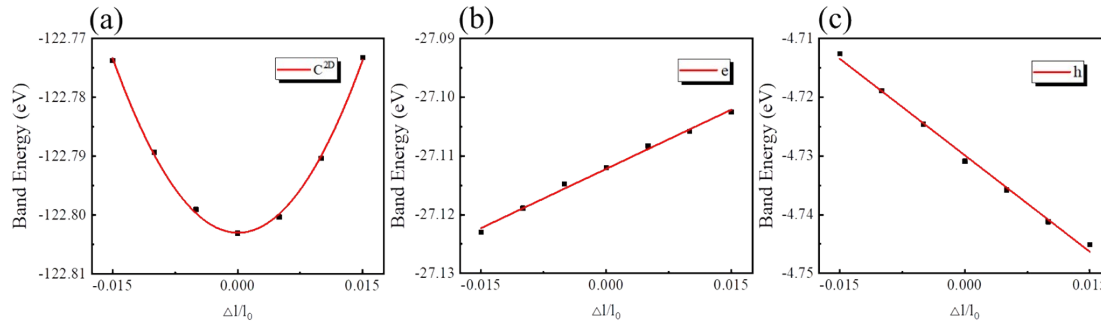


Fig. S1. Variation in total energy (a) and VBM/CBM energy (b, c) for Janus BiSbC_3 monolayer with strain along the X direction.

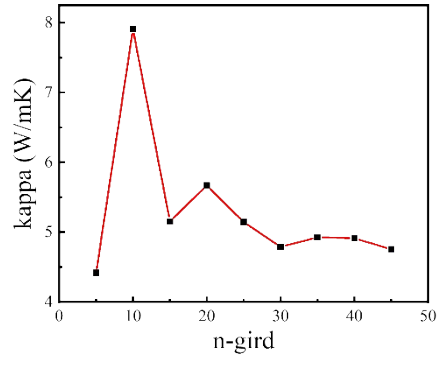


Fig. S2. Convergence tests of lattice thermal conductivity κ_l of n -grid for the Janus BiSbC₃ monolayer.

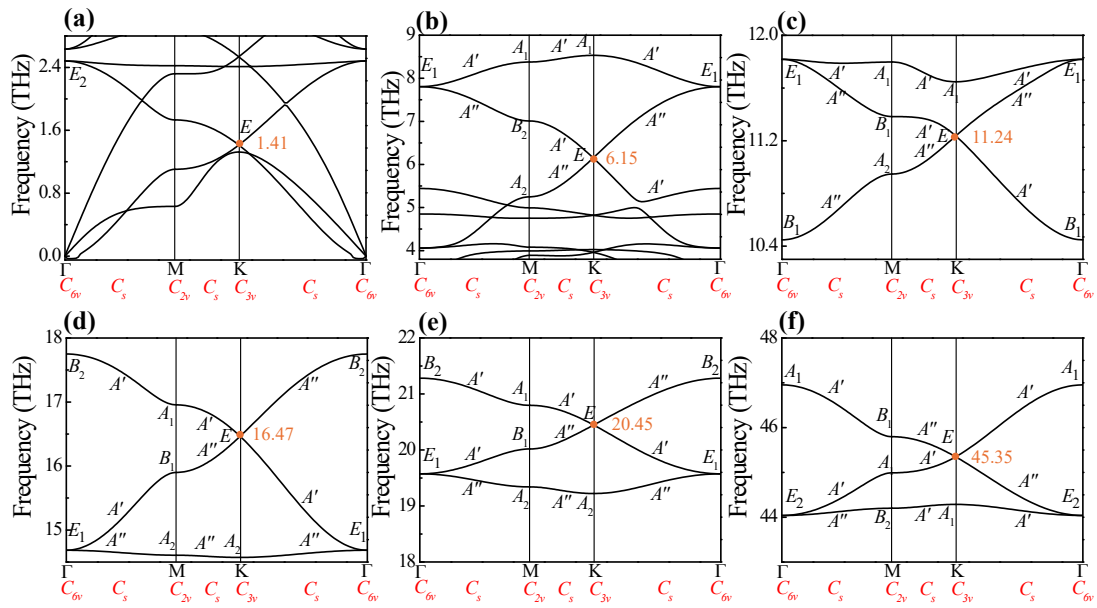


Fig. S3. Point group of phonon dispersion curves in 0-2.8 THz (a), 4-9 THz (b), 10.4-12 THz (c), 14-18 THz (d), 18-22 THz (e) and 43-48 THz (f) along the high-symmetry lines of the first Brillouin zone for Janus BiSbC₃ monolayer.

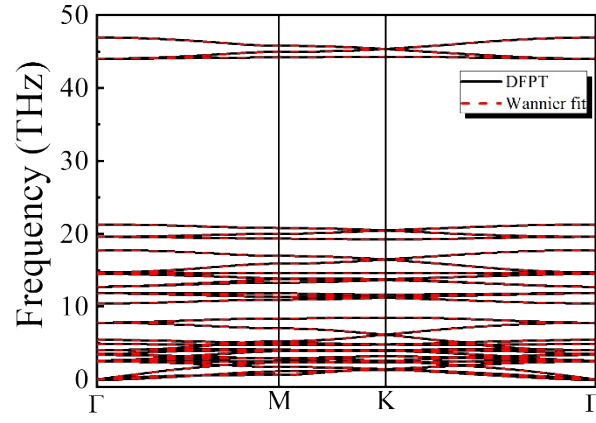


Fig. S4. Phonon dispersion curve of the Janus BiSbC₃ monolayer, with results from DFPT (black) and Wannier fit (red).

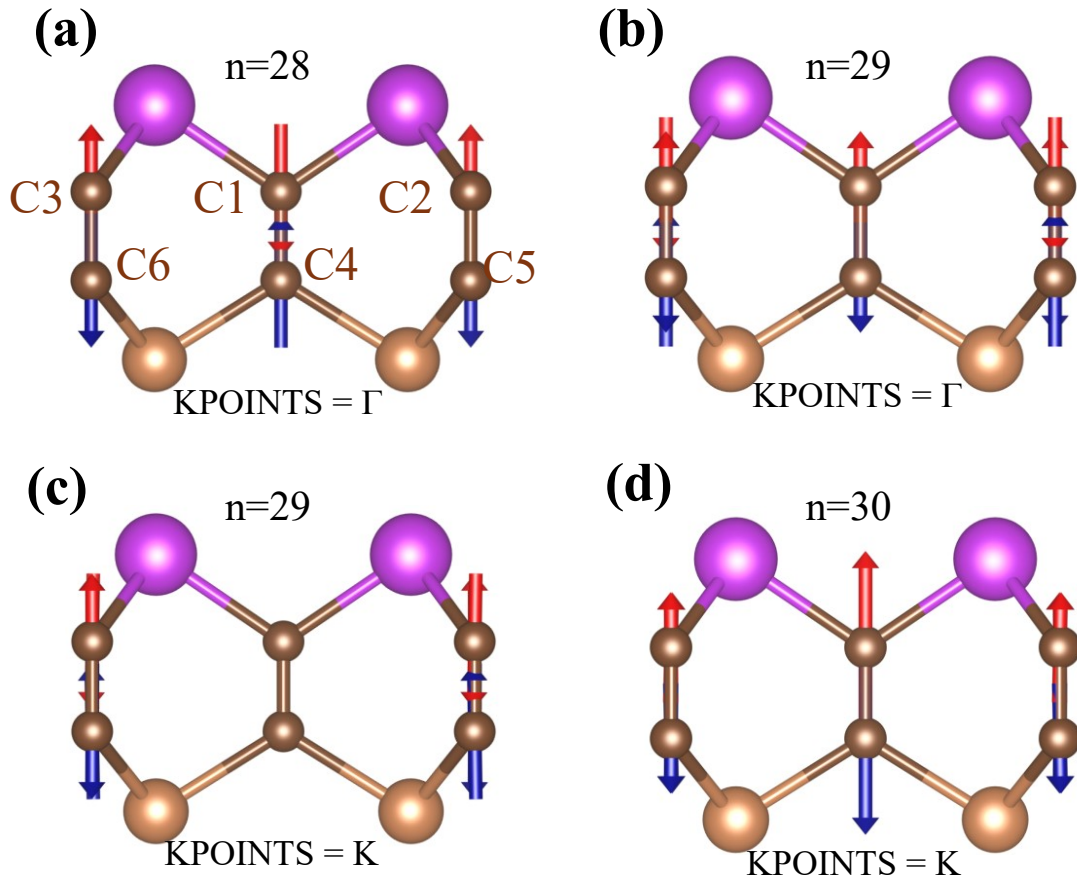


Fig. S5. Lattice vibrational modes of the Janus BiSbC₃ monolayer along the Γ -point and K-point. (a-b) The 28th and 29th phonon branches along the Γ -point, (c-d) the 29th and 30th phonon branches along the K-point.

Table. S1. Character for point group of phonon dispersion curves along the high-symmetry lines of the first Brillouin zone for Janus BiSbC₃ monolayer.

	C_{6v} $h=12$						C_{2v} $h=4$				C_{3v} $h=6$			C_s $h=2$	
	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$	E	C_2	σ_v	σ_d	E	$2C_3$	$3\sigma_v$	E	σ_h
A_1	1	1	1	1	1	1	A_1	1	1	1	A_1	1	1	A'	1
A_2	1	1	1	1	-1	-1	A_2	1	1	-1	A_2	1	1	A''	-1
B_1	1	-1	1	-1	1	-1	B_1	1	-1	1	E	2	-1		
B_2	1	-1	1	-1	-1	1	B_2	1	1	1					
E_1	2	1	-1	-2	0	0									
E_2	2	-1	-1	2	0	0									