Supplementary Material

Anisotropic Thermal and Electrical Transport Properties Induced High Thermoelectric Performance in $Ir_2Cl_2O_2$ Monolayer

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1. Phonon Vibrational Mode

As shown in Figure 2 in main text, ZA and TA modes narrow down and become almost degenerate in the X-Y path. Similar phenomena can be observed between LA and the lowest optical branch. This implies that strong coupling exists in acoustic-acoustic and acoustic-optical modes, leading to low thermal conductivity. Similar phenomena can

be observed between LA and the lowest optical branch. Through visualization technology, we obtain the vibration modes of high symmetry points on the degenerate phonon band, as shown in the following figures. The doubly degenerate phonon band of ZA/TA is associated with the $E`$ mode and that of LA/Opt is the $E``$ mode. 'E' indicates that the representation is double-degenerate. The prime (`) and double prime (``) in the symmetry representation label represents symmetric or anti-symmetric with respect to a mirror plane horizontal to the principal rotational axis.

Table S1 The corresponding relationship between the supplementary picture, energy band, high symmetry point and view plane.

Band	ZA/TA degenerate band									LA/Opt degenerate band								
Point	X			S			Y			X			S			Y		
Plane	*bc*	*ac*	*ab*	*bc*	*ac*	*ab*	*bc*	*ac*	*ab*	*bc*	*ac*	*ab*	*bc*	*ac*	*ab*	*bc*	*ac*	*ab*
Figure	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	S16	S17	S18