Supplemental Material

Giant effect of spin-lattice coupling on the thermal transport

in two-dimensional ferromagnetic CrI₃

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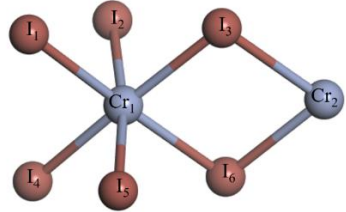
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Table SI: The lattice constant, bond lengths and bond angles for CrI_3 in PM and FM states are listed, respectively. The labeled structure diagram is also presented.

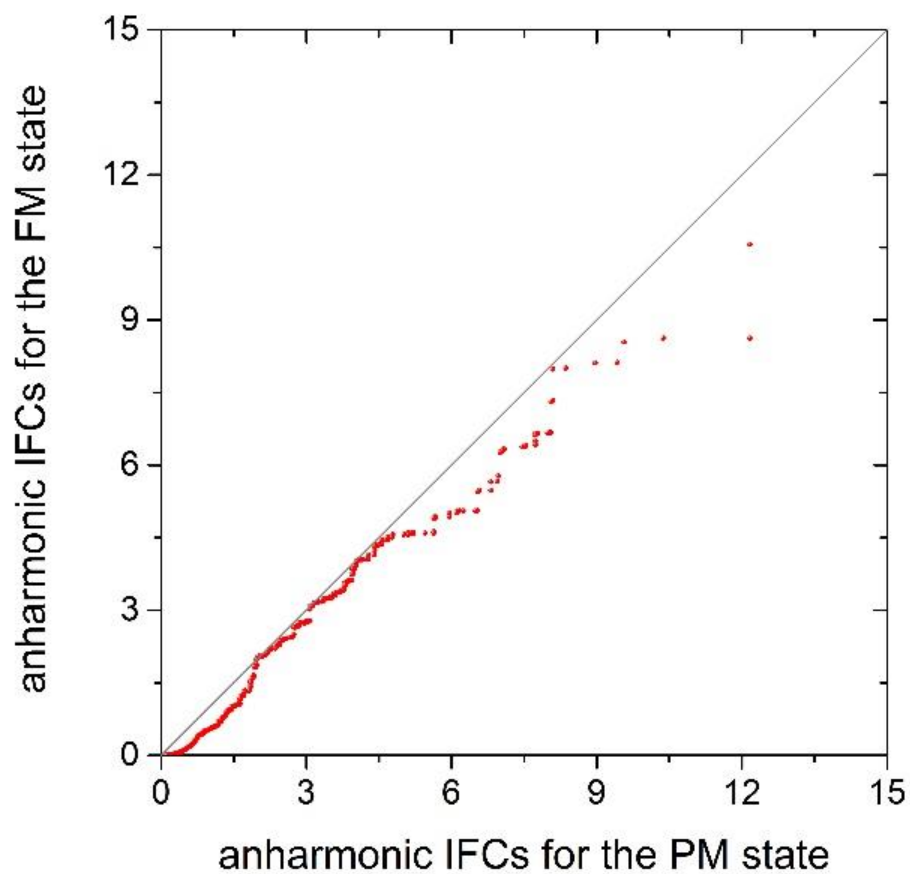| PM		FM		Side view of the structure
a, b (Å)	6.992	a, b (Å)	7.003	
Cr_1-$I_{1/2/3}$ (Å)	2.67227	Cr_1-$I_{1/2/3}$ (Å)	2.73721	
Cr_1-$I_{4/5/6}$ (Å)	2.67215	Cr_1-$I_{4/5/6}$ (Å)	2.73715	
Cr_1-Cr_2 (Å)	4.037	Cr_1-Cr_2 (Å)	4.403	
$\angle I_1Cr_1I_3$, $\angle I_1Cr_1I_2$, $\angle I_2Cr_1I_3$	90.947°	$\angle I_1Cr_1I_3$, $\angle I_1Cr_1I_2$, $\angle I_2Cr_1I_3$	90.625°	
$\angle I_4Cr_1I_5$, $\angle I_5Cr_1I_6$, $\angle I_4Cr_1I_6$	90.955°	$\angle I_4Cr_1I_5$, $\angle I_5Cr_1I_6$, $\angle I_4Cr_1I_6$	90.630°	
$\angle I_1Cr_1I_2$	81.898°	$\angle I_1Cr_1I_2$	84.786°	

Figure S1: The comparison of anharmonic IFCs between FM and PM phases (red scatter plot). The solid grey line with a slope of 1 is plotted for clear comparison.
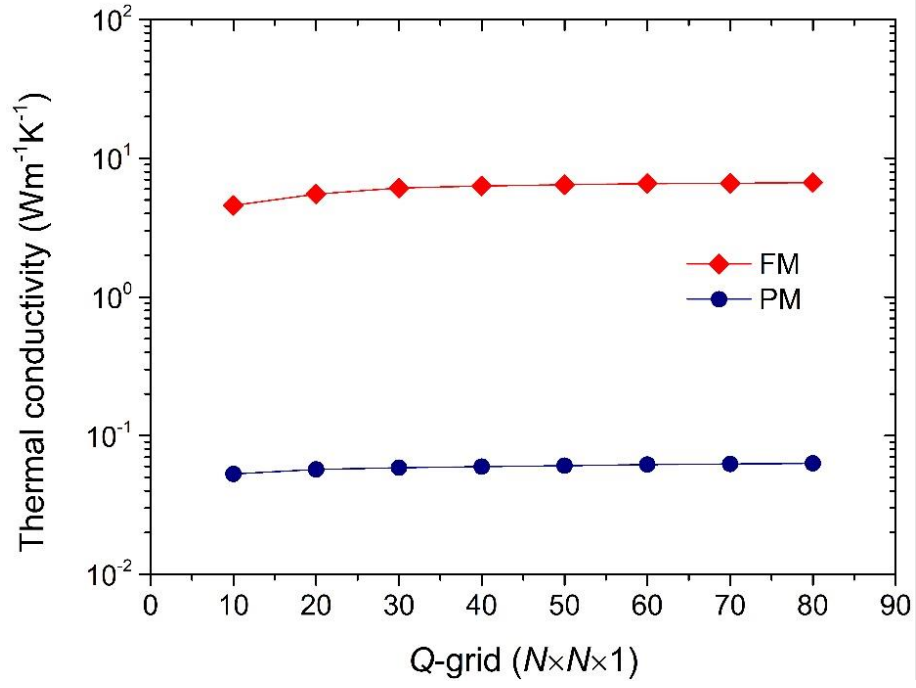
Figure S2: The test curve of interrogation grid (N×N×1) on the thermal conductivity calculation for CrI$_3$ in FM and PM states. In our calculations, 70×70×1 is chosen to achieve the converged thermal conductivity.
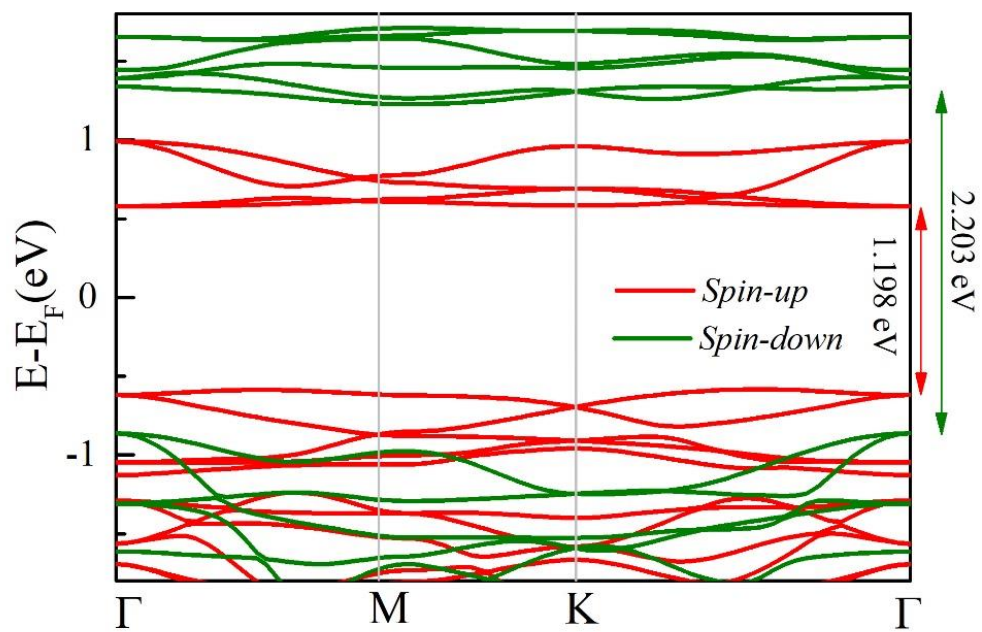
Figure S3: The calculated band structure for ferromagnetic CrI$_3$. The red and green bands represent the spin-up and spin-down electronic states.