Investigation of Lattice Thermal Transport Properties of Janus XClO (X=Cr, Ir) Monolayer by First-principles Calculations

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Supplementary Information (SI)

The structure coordination of CrClO unit cell:

```
1.0
        3.8887500763    0.0000000000    0.0000000000
        0.0000000000    3.2132298946    0.0000000000
        0.0000000000    0.0000000000   20.0000000000
   Cr   Cl   O
    2    2   2
Direct
     0.500000000     0.500000000     0.542909050
    -0.000000000    -0.000000000     0.457090998
     0.000000000     0.500000000     0.372164011
     0.500000000    -0.000000000     0.627835989
     0.500000000    -0.000000000     0.479659986
    -0.000000000     0.500000000     0.520340014
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The structure coordination of IrClO unit cell:

1.0

4.0859198570	0.0000000000	0.0000000000
0.0000000000	3.3764901161	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Ir	Cl	O
2	2	2

Direct

0.500000000	0.500000000	0.545497990
-0.000000000	-0.000000000	0.454502010
-0.000000000	0.500000000	0.375256014
0.500000000	-0.000000000	0.624743986
0.500000000	-0.000000000	0.478155994
0.000000000	0.500000000	0.521844006

The structure coordination of CrIrClO unit cell:

1.0

4.0170898438	0.0000000000	0.0000000000
0.0000000000	3.2956500053	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Cr	Ir	Cl	O
1	1	2	2

Direct

0.500000000	0.500000000	0.541862011
-0.000000000	-0.000000000	0.455716038
-0.000000000	0.500000000	0.374339008
0.500000000	0.000000000	0.625345993
0.500000000	-0.000000000	0.479332018
-0.000000000	0.500000000	0.523405027