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

Supporting Information

Two-Dimensional Ferroelastic Semiconductors in Single-Layer Indium Oxygen Halide InOY (Y=Cl/Br)

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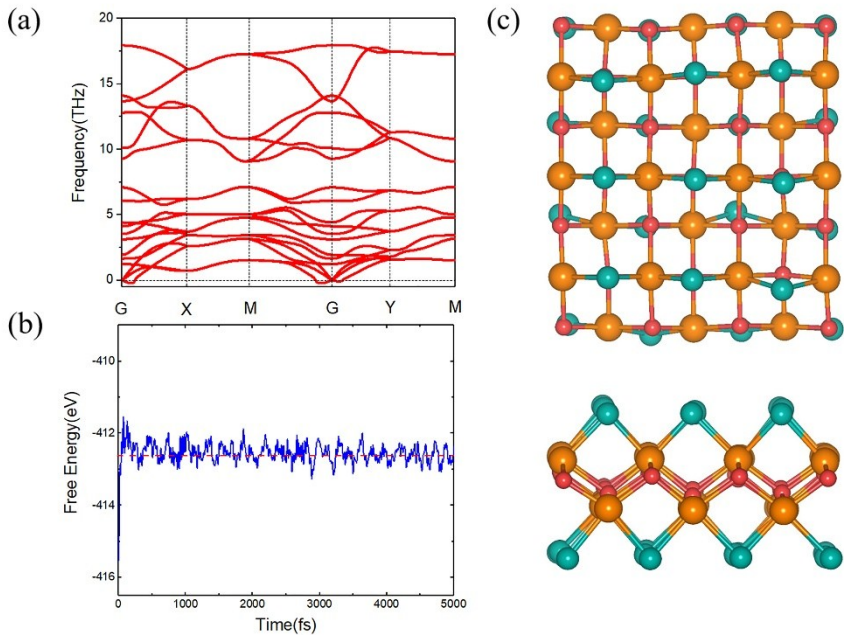

Fig. S1. (a) The phonon bands of SL InOBr. (b) The variation of total energy during AIMD (500 K, 5 ps) simulations. (c) Crystal structure of SL InOCl taken from the end of AIMD.

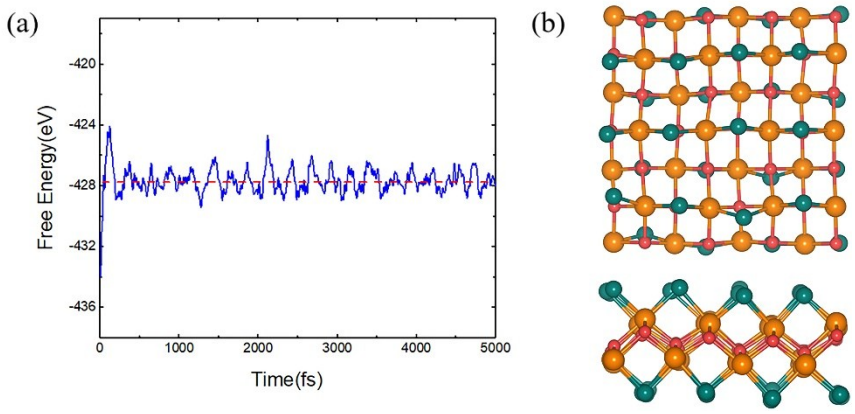

Fig. S2. (a) The variation of total energy during AIMD (500 K, 5 ps) simulations. (b) Crystal structure of SL InOCl taken from the end of AIMD.

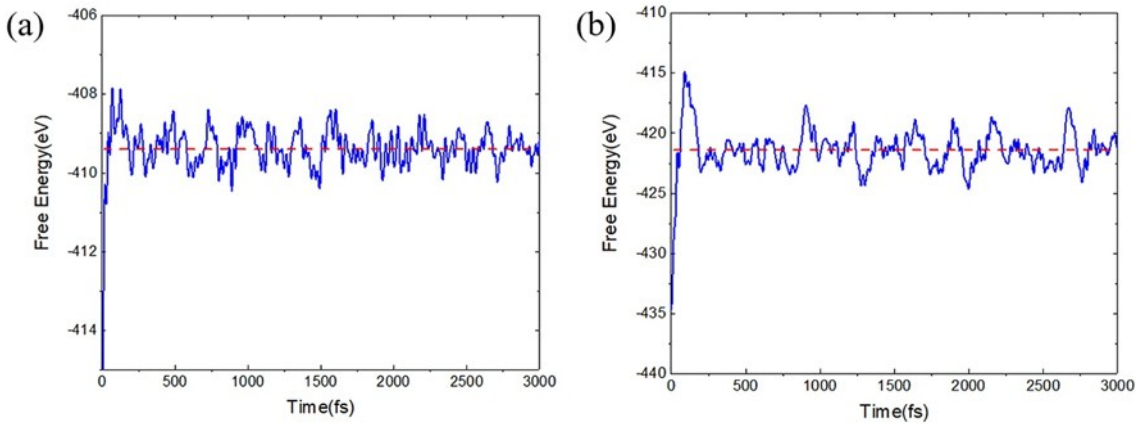

Fig. S3. The variation of total energy during AIMD (1000 K, 3 ps) simulations of InOBr (a), InOCl (b).

We perform the AIMD simulations in Fig. S1, Fig. S2 and Fig. S3. For the AIMD simulation (5 ps at 500 K and 3 ps at 1000K), neither of InOCl and InOBr broken bond nor geometry reconstruction is observed for both systems; see Fig. S2b and Fig. S1c. And the fluctuation of total energy is shown in Fig. S2a and Fig. S1b. These results confirm that SL InOY is thermally local minimal.

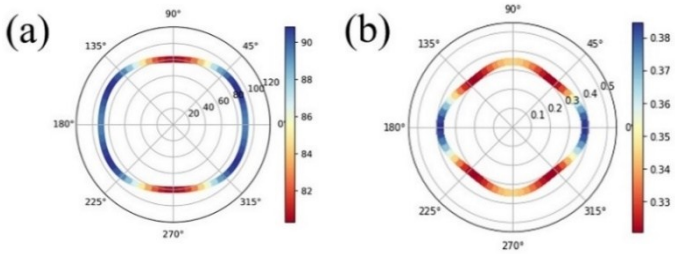

Fig. S4. (a) Young's modulus and (b) Poisson's ration of InOBr as a function of the angle θ. θ = 0º corresponds to the a axis.

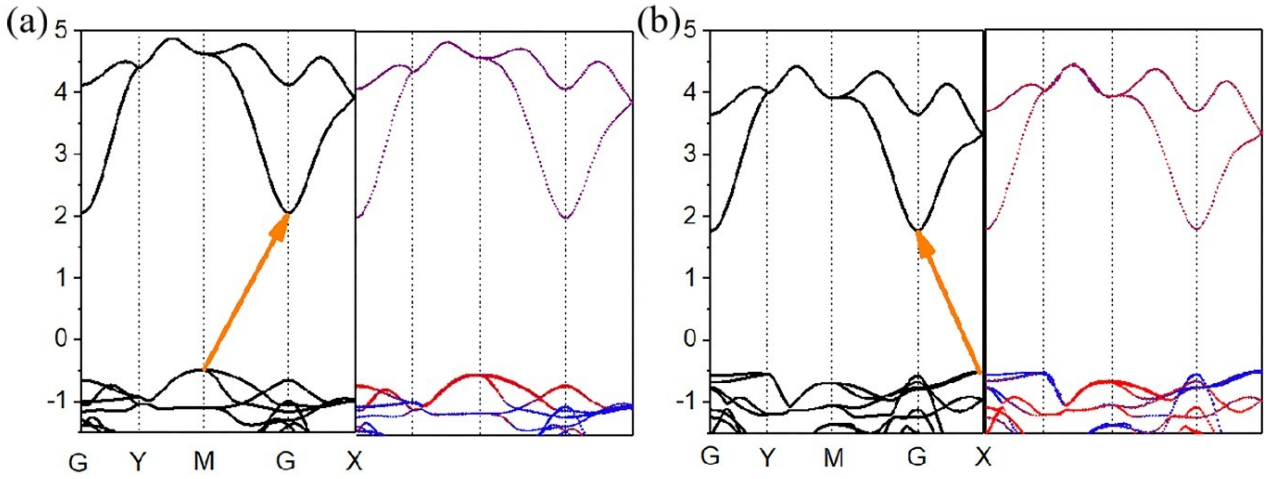

Fig. S5. The band structure and the fat band structure of InOCl (a) and InOBr (b). Purple: In; Red: O; Blue: Cl or Br.

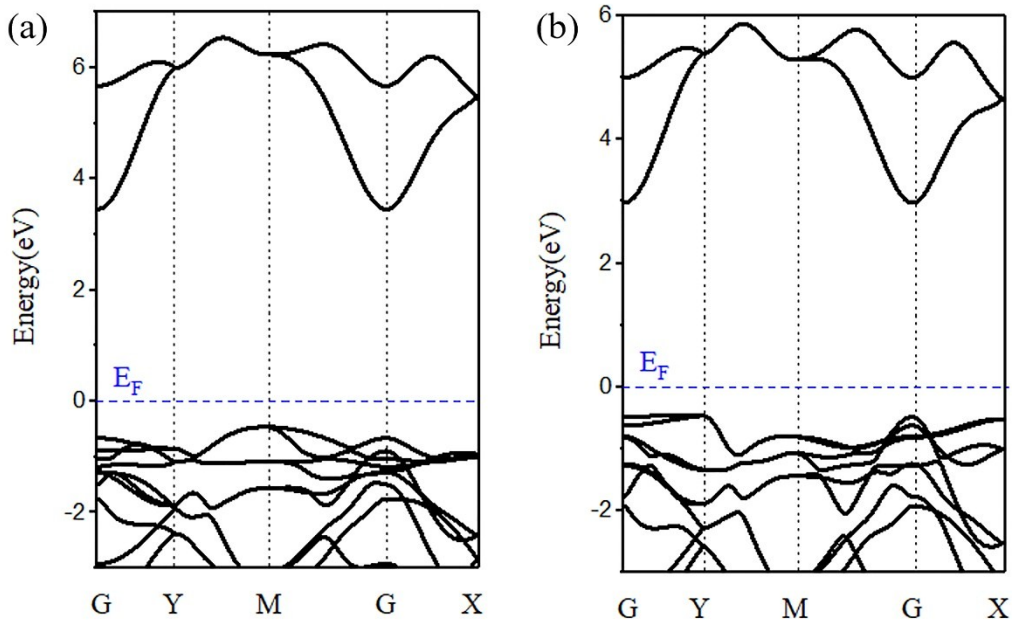

Fig. S6. The band structures of SL InOCl (a) and InOBr (b) calculated by the HSE06 method.

The lattice parameters and atomic position coordinates SL InOYs.

InOCl

a	3.5738492593467126	0.0000000000000000	0.0000000000000000
b	0.0000000000000000	4.2070566146559161	0.0000000000000000
c	0.0000000000000000	0.0000000000000000	21.0560965682156862

O	0.25	0.25	0.4823615354942151
O	0.75	0.75	0.5176384645057849
Cl	0.75	0.75	0.3650538220037595
Cl	0.25	0.25	0.6349461779962405
In	0.75	0.25	0.5476018644370646
In	0.25	0.75	0.4523981355629353

InOBr

a	3.6753612768970489	0.0000000000000000	0.0000000000000000
b	0.0000000000000000	4.1847440686720478	0.0000000000000000
c	0.0000000000000000	0.0000000000000000	21.7182952632748005

O	0.25	0.25	0.4849400114956369
O	0.75	0.75	0.5150599885043630
Br	0.75	0.75	0.3624338252215629
Br	0.25	0.25	0.6375661747784370
In	0.75	0.25	0.5459760384390236
In	0.25	0.75	0.4540239615609769