

Supporting information

Strain-engineering enables reversible semiconductor-metal transition of skutterudite IrAs₃

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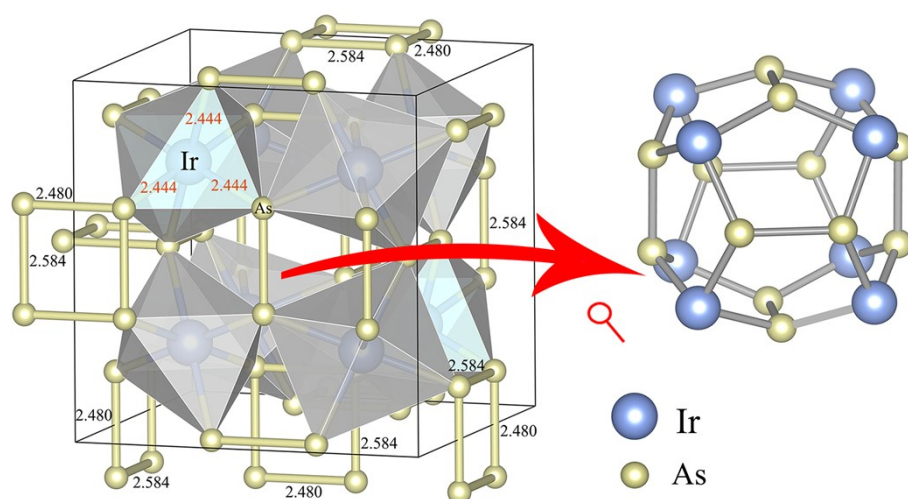


Fig. S1 The icosahedral cage formed by the Ir and As atoms in IrAs_3 .

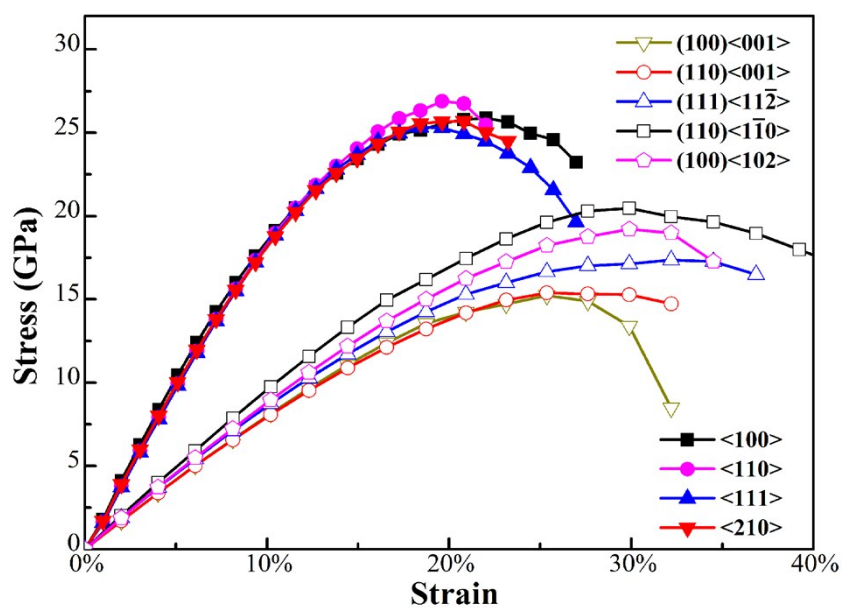


Fig. S2 Stress-strain curves of IrAs_3 along a plurality of high-symmetry directions under tensile and shear deformation.

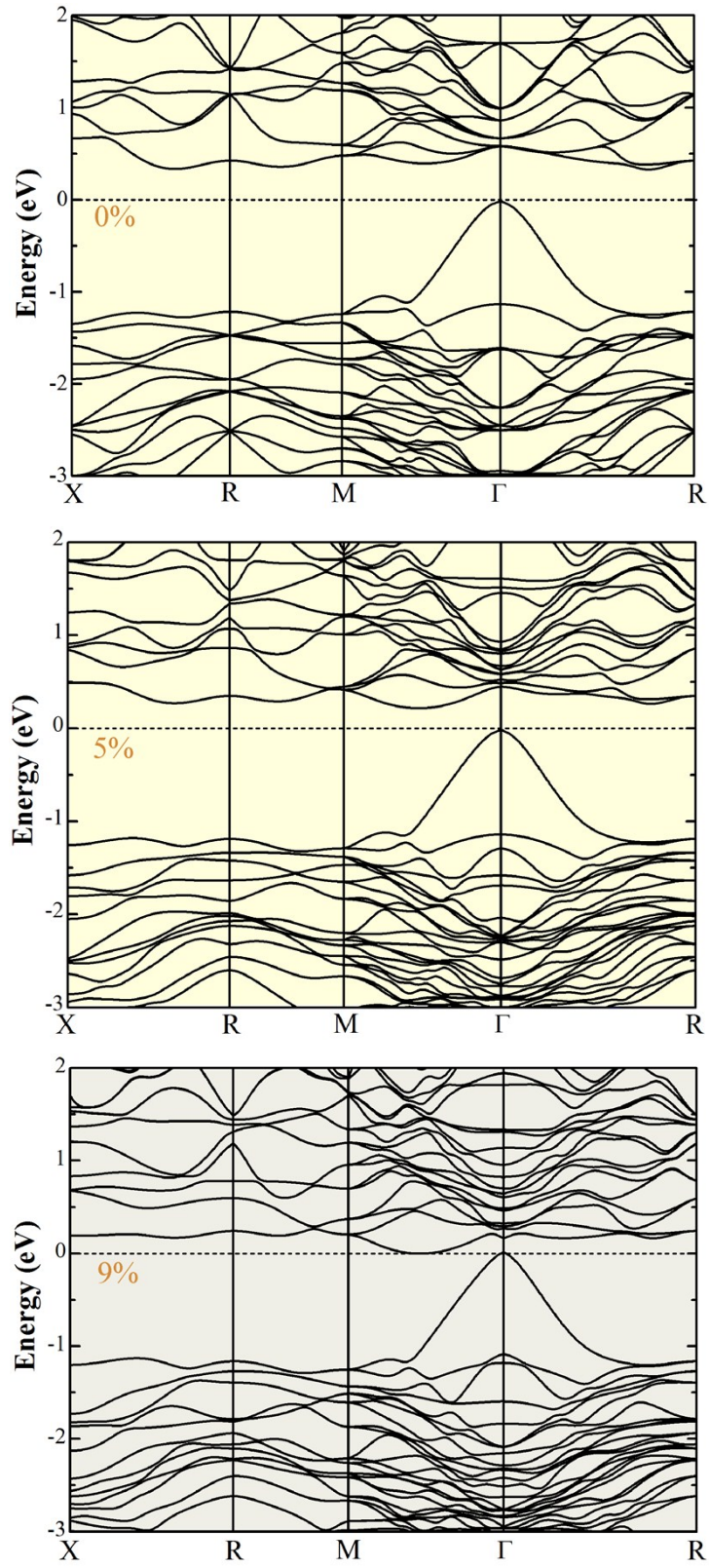


Fig. S3 Electronic band structures of IrAs₃ at 0%, 5% and ~9% tensile strain. The fermi level has been set to the energy zero.

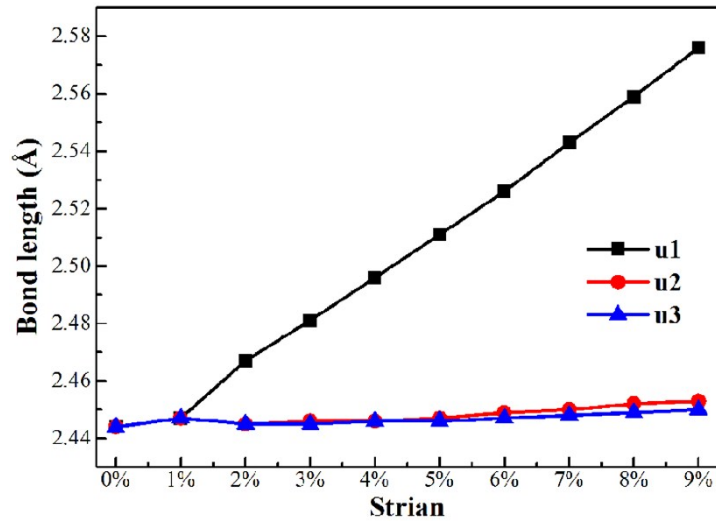


Fig. S4 Strain-induced bond length variation of Ir-As bond in the direction of u_1 , u_2 , and u_3 .

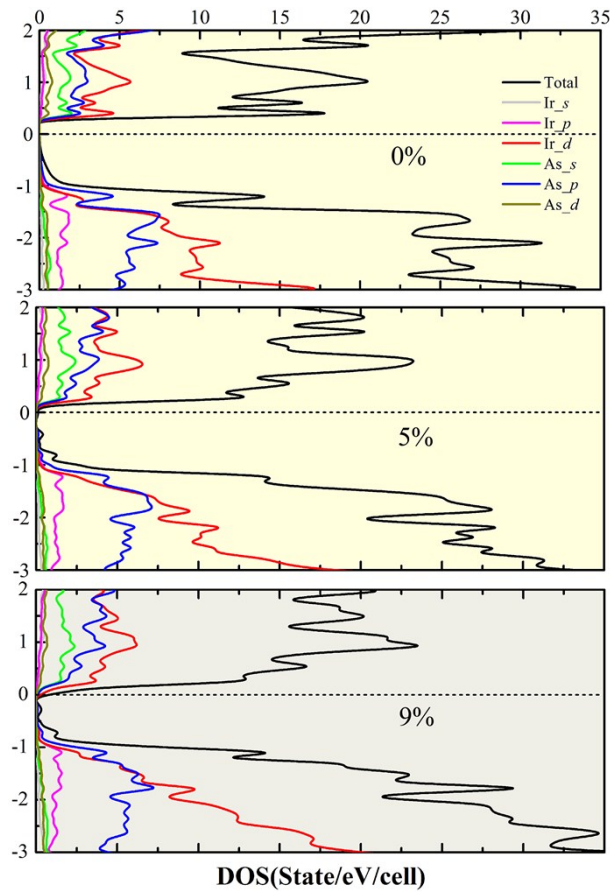


Fig. S5 Total density of states (DOS) and projected densities of states (PDOSs) of Ir and As for IrAs_3 at 0%, 5% and ~9% tensile strain. The fermi level has been set to the energy zero.

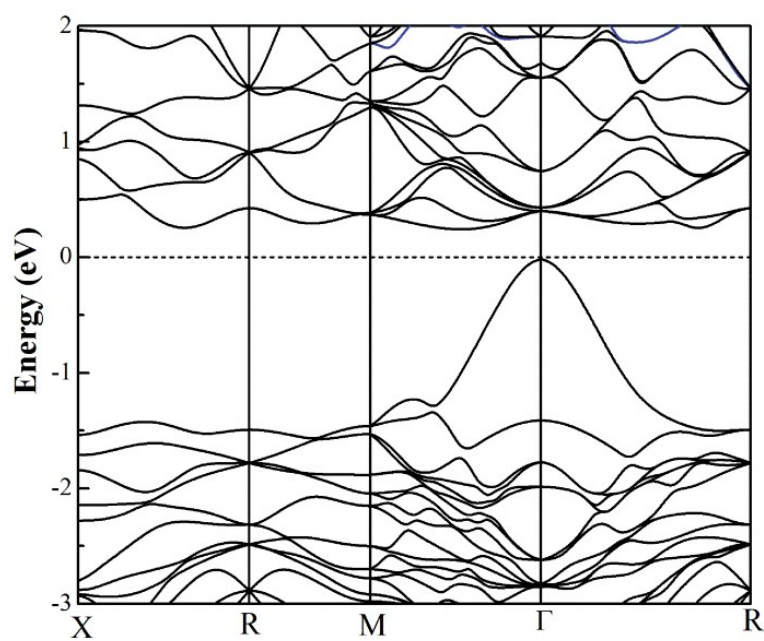


Fig. S6 Electronic band structure of IrAs₃ at 20 GPa. The horizontal dashed line indicates the Fermi level.

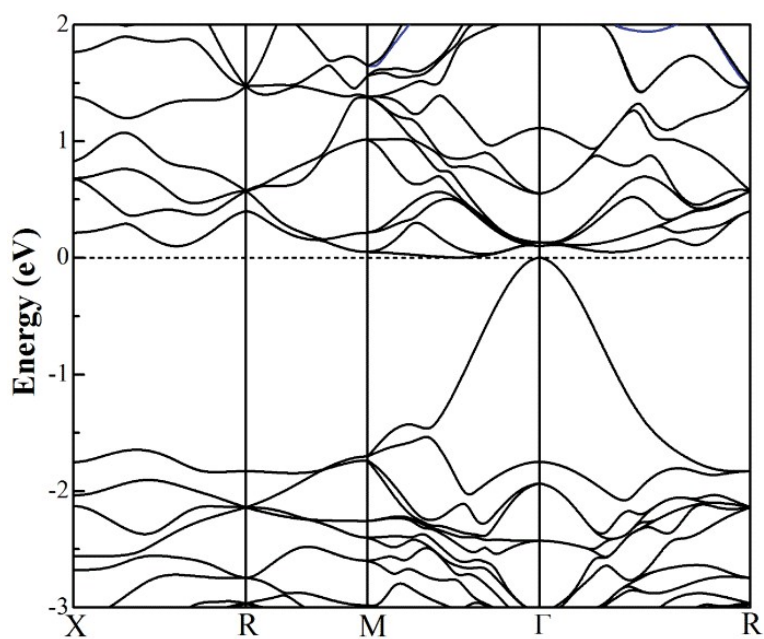


Fig. S7 Electronic band structure of IrAs₃ at 53.5 GPa. The horizontal dashed line indicates the Fermi level.

Structural information of IrAs₃ in this text

IrAs₃

1.0

8.4690999985	0.0000000000	0.0000000000
0.0000000000	8.4690999985	0.0000000000
0.0000000000	0.0000000000	8.4690999985

Ir As

8 24

Direct

0.250000000	0.250000000	0.250000000
0.750000000	0.750000000	0.750000000
0.750000000	0.750000000	0.250000000
0.250000000	0.250000000	0.750000000
0.750000000	0.250000000	0.750000000
0.250000000	0.750000000	0.250000000
0.250000000	0.750000000	0.750000000
0.750000000	0.250000000	0.250000000
0.000000000	0.350019991	0.150010005
0.000000000	0.649980009	0.849990010
0.000000000	0.649980009	0.150010005
0.000000000	0.350019991	0.849990010
0.150010005	0.000000000	0.350019991
0.849990010	0.000000000	0.649980009
0.150010005	0.000000000	0.649980009
0.849990010	0.000000000	0.350019991
0.350019991	0.150010005	0.000000000
0.649980009	0.849990010	0.000000000
0.649980009	0.150010005	0.000000000

0.350019991	0.849990010	0.000000000
0.500000000	0.850019991	0.650009990
0.500000000	0.149980009	0.349990010
0.500000000	0.149980009	0.650009990
0.500000000	0.850019991	0.349990010
0.650009990	0.500000000	0.850019991
0.349990010	0.500000000	0.149980009
0.650009990	0.500000000	0.149980009
0.349990010	0.500000000	0.850019991
0.850019991	0.650009990	0.500000000
0.149980009	0.349990010	0.500000000
0.149980009	0.650009990	0.500000000
0.850019991	0.349990010	0.500000000