Supplementary Information for

Predicted high thermoelectric performance in two-dimensional Indium Telluride and its dependence against strain

Min-Shan Li[1,4], Kai-Xuan Chen[3,4], Dong-Chuan Mo[2,4,a)], Shu-Shen Lyu[2,4]

[1] *School of Chemical Engineering and Technology, Sun Yat-sen University, No.135, Xingang Xi Road, Guangzhou, 510275, P. R. China*

[2] *School of Materials, Sun Yat-sen University, No. 135, Xingang Xi Road, Guangzhou, 510275, P. R. China*

[3] *Chair of Solid-State and Quantum Chemistry, Institute of Inorganic Chemistry, RWTH Aachen University, 52056 Aachen, Germany*

[4] *Guangdong Engineering Technology Research Centre for Advanced Thermal Control Material and System Integration (ATCMSI), Sun Yat-sen University, No. 135, Xingang Xi Road, Guangzhou, 510275, P. R. China*

Table S1. Structural parameters for 2D *MX* (*M*=Ga, In and *X*=S, Se, Te) monolayers, including lattice constant (a), bond length (d_{MM} and d_{MX}), layer thickness (δ) and bond angle (θ_1 and θ_2), as depicted in Fig. 1.

	a/ Å	d_{MM}/ Å	d_{MX}/ Å	δ/ Å	θ_1/ deg	θ_2/ deg
GaS	3.629	2.472	2.360	4.645	117.4	100.5
GaSe	3.813	2.469	2.496	4.820	118.1	99.60
GaTe	4.130	2.467	2.704	5.019	118.2	99.56
InS	3.924	2.825	2.553	5.179	117.5	100.4
InSe	4.086	2.822	2.682	5.371	118.4	99.26
InTe	4.387	2.814	2.884	5.571	118.6	99.04

[a)] Electronic mail: modongch@mail.sysu.edu.cn

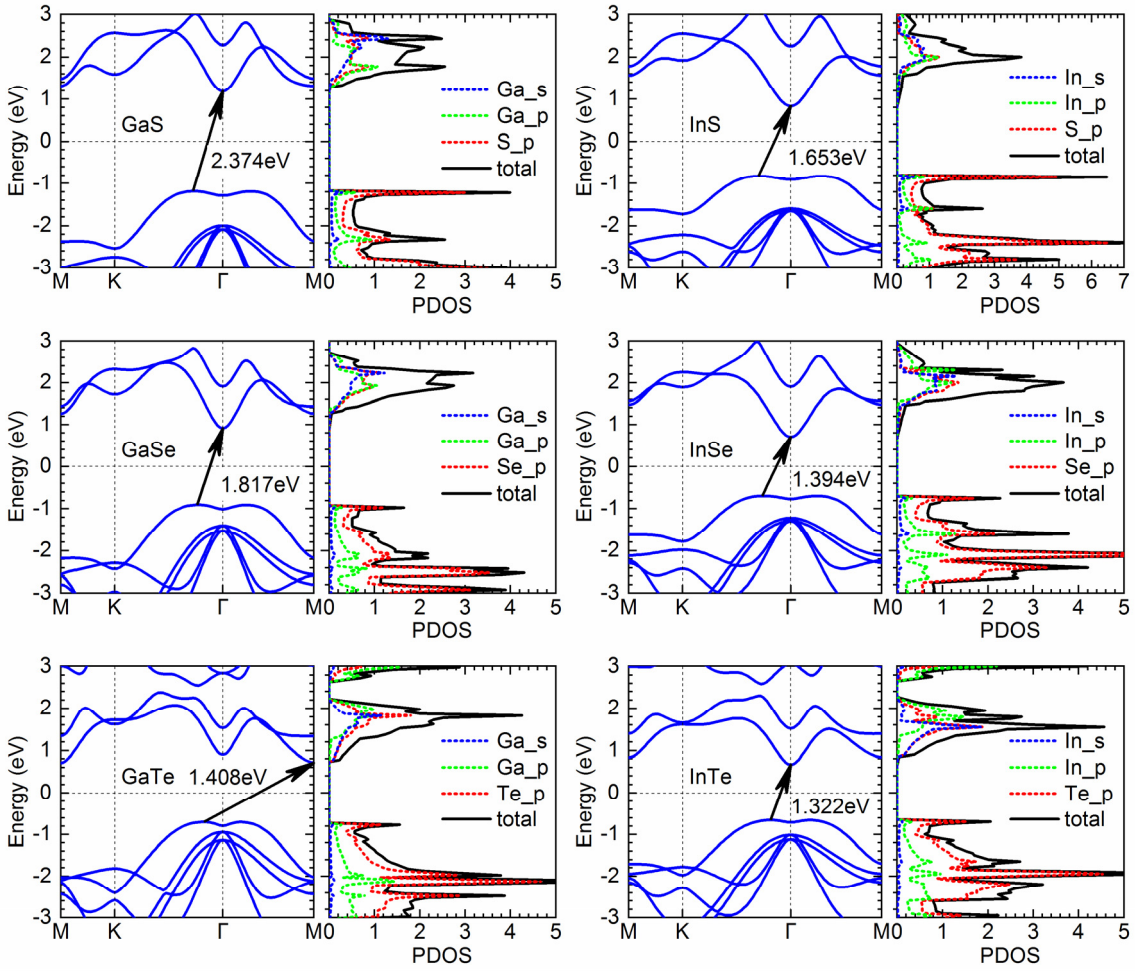

Figure S1. Electronic band structures and projected density of states (DOS) for *MX* (*M*=Ga, In and *X*=S, Se, Te) monolayers.

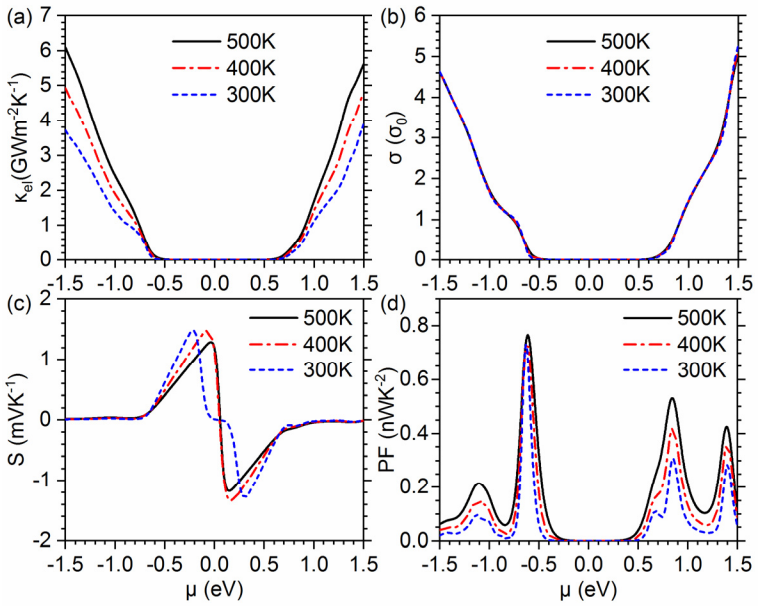

Figure S2. (a) Electronic thermal conductance κ_{el}, (b) electronic conductance σ, (c) Seebeck coefficient S and (d) power factor PF as functions of chemical potential μ for InTe monolayers at diffreent temperatures.

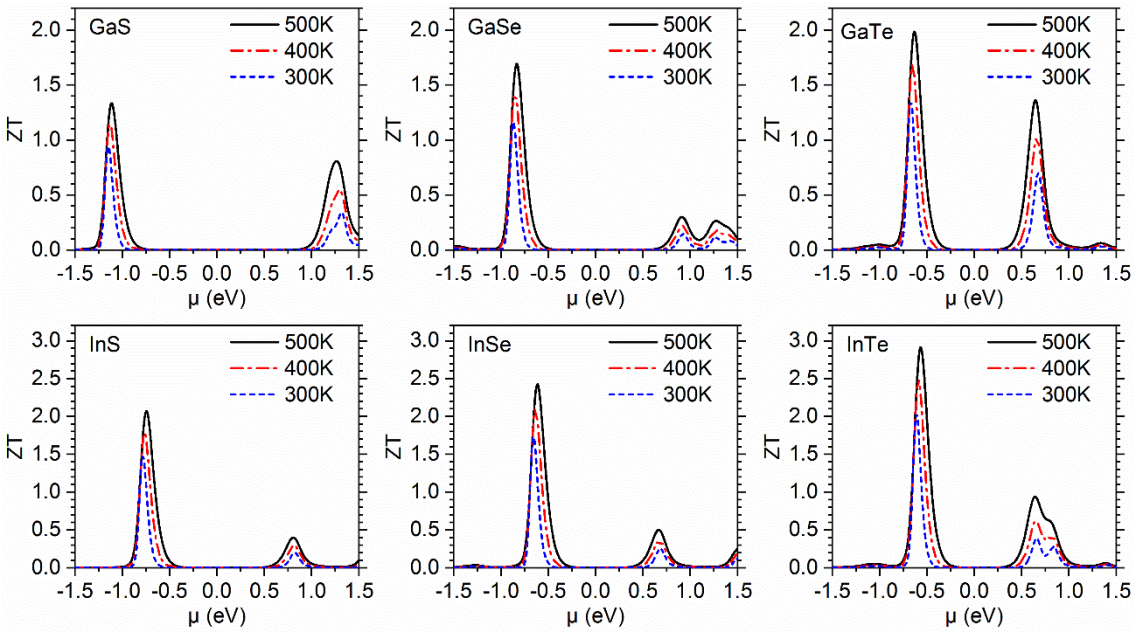

Figure S3. ZT value for MX (M=Ga, In and X=S, Se, Te) monolayers as a function of chemical potential μ at diffreent temperatures.

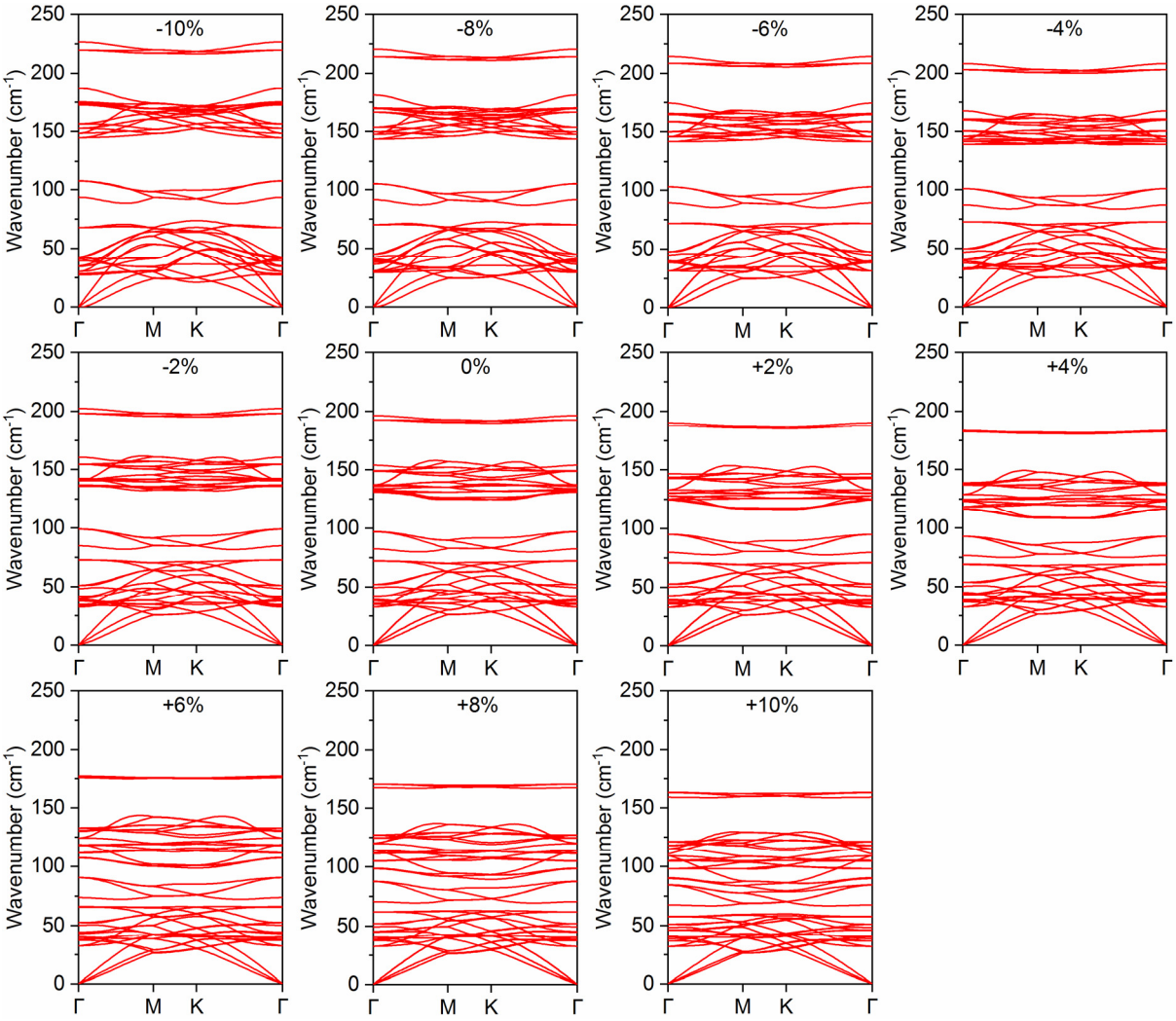

Figure S4. Phonon dispersions for InTe monolayer under biaxial lattice strain from -10% to +10%. Absence of imaginary phonon vibration modes confirms the dynamical stability of 2D InTe under biaxial strain from -10% to +10%.

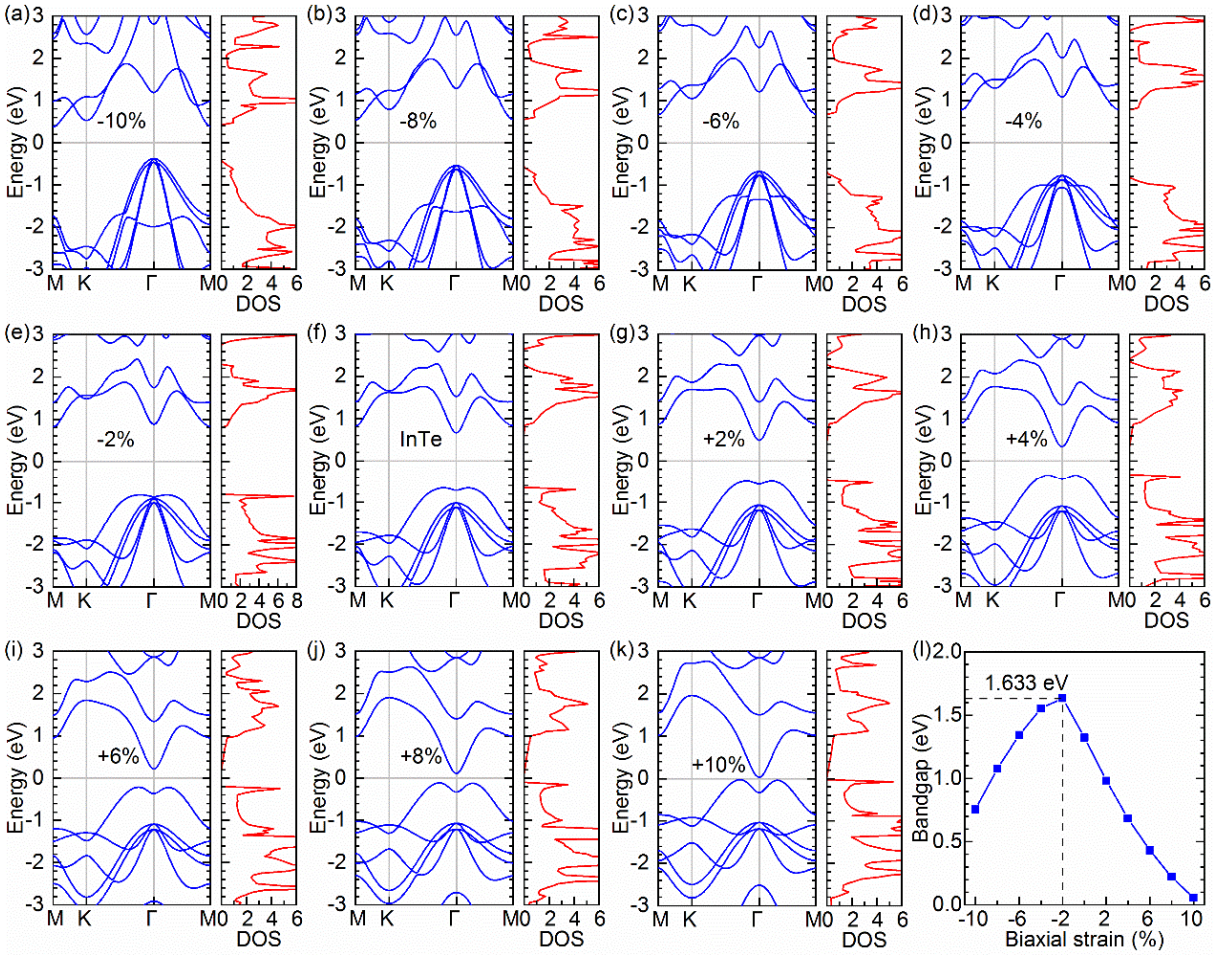

Figure S5. (a-k) Electronic band structures and density of states (DOS) and (l) electronic band gap for InTe monolayer under biaxial lattice strain from -10% to +10%. InTe monolayer has the largest bandgap of 1.633 eV under -2% compressive strain.