Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Prediction of Strain-induced Phonon-mediated Superconductivity in Monolayer YS

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Details of structure evolvement

Our structural prediction approach is based on a global minimization of free energy surfaces of given compounds by combining ab initio total-energy calculations with the particle swarm optimization (PSO) algorithm. The structure search of YS monolayer is performed with simulation cells containing 1−8 formula units. In the first generation, a population of structures belonging to certain space group symmetries are randomly constructed. Local optimizations of candidate structures are done by using the conjugate gradients method through the VASP code, with an economy set of input parameters and an energy convergence threshold of 1×10^{-5} eV per cell. Starting from the second generation, 70% structures in the previous generation with the lower enthalpies are selected to produce the structures of next generation by the PSO operators. The 30% structures in the new generation are randomly generated. A structure fingerprinting technique of bond characterization matrix is employed to evaluate each newly generated structure, so that identical structures are strictly forbidden. These procedures significantly enhance the diversity of sampled structures during the evolution, which is crucial in driving the search into the global minimum.

Table. S1 Calculated lattice parameters (space group and lattice constants), atomic positions and Bader charge for *t*-YS.

Phase	Lattice parameters	Atomic Position	Bader charge (e)

YS (*P4/nmm*)	a = b = 3.81	Y (2c) (0, 0.5, 0.43460)	+1.50
		S (2c) (0, 0.5, 0.59378)	-1.50

Table. S2 Calculated atomic vibrations for each mode of *t*-YS.

Phase	Mode	$\omega\ (cm^{-1})$	Active
YS	E	152.9	I+R
	A1	163.8	R
	A1	219.0	R
	B2	261.4	I+R
	E	264.6	I+R
	E	294.0	I+R

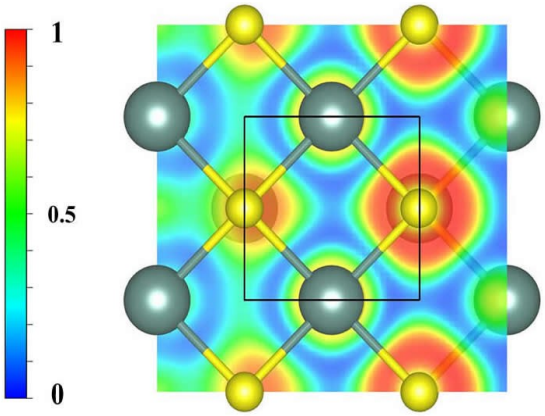

Fig. S1 Maps of the electron localization function (ELF) with a scale bar from 0 to 1 for *t*-YS.

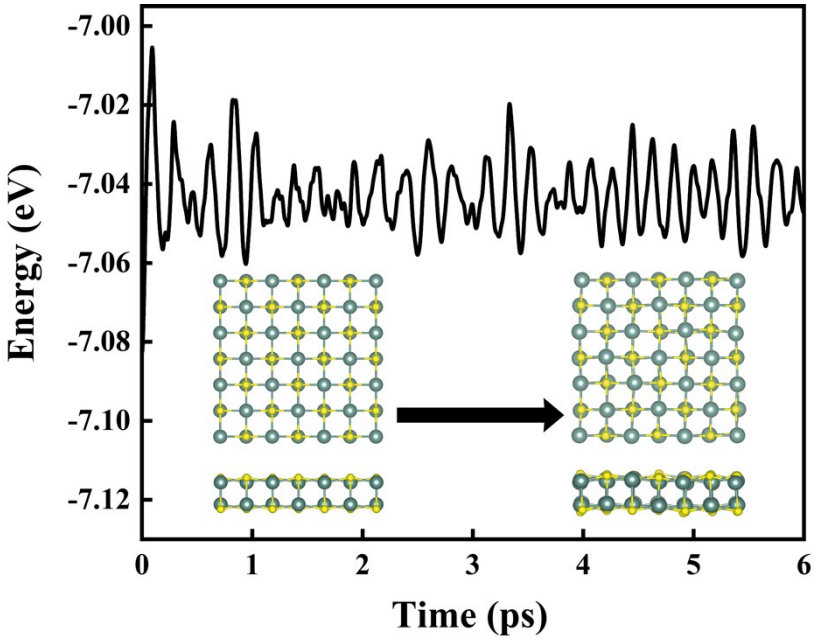

Fig. S2 Snapshots of the final frame of *t*-YS at temperatures of 300 K at the end of 6 ps AIMD simulations.

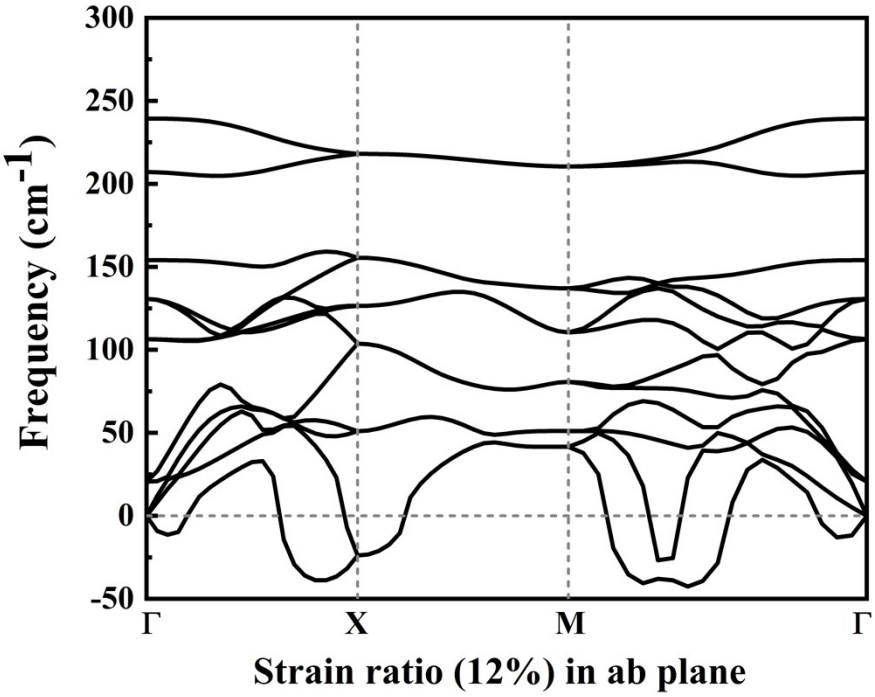

Fig. S3 Phonon frequency dispersion under tensile strain of 12% for *t*-YS.

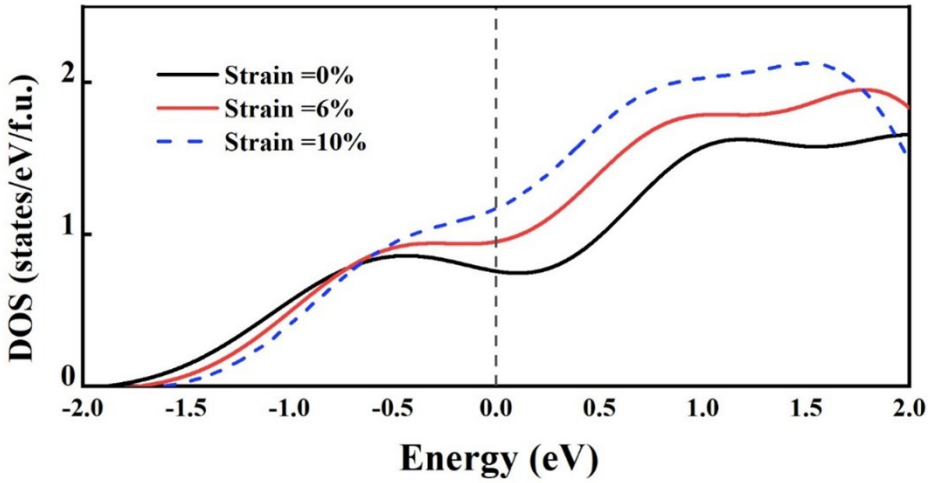

Fig. S4 Density of states (DOS) under strain of 0% (solid black lines), 6% (solid red lines) and 10% (dashed blue lines), respectively.

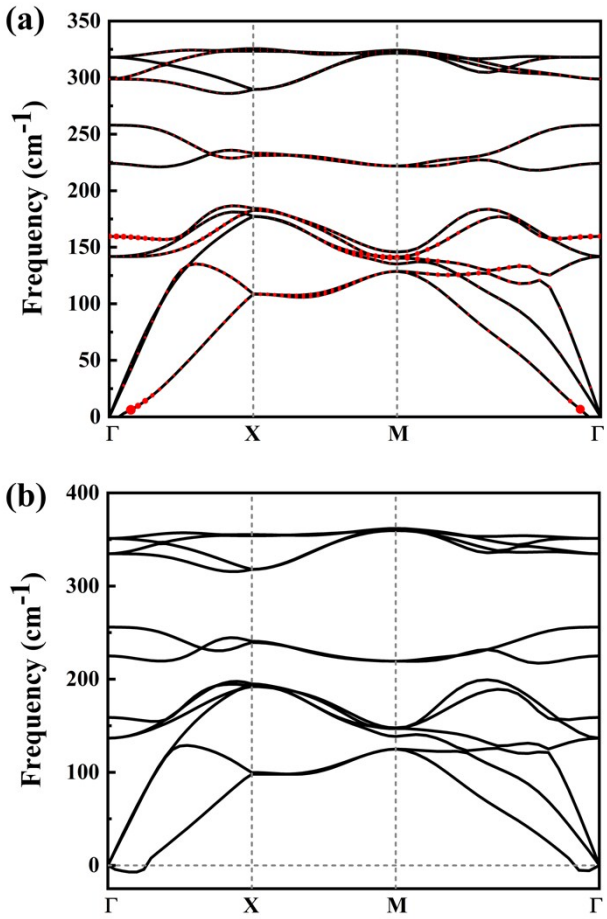

Fig. S5 Phonon frequency dispersions under biaxial compressive strain of (a) 2% and (b) 4% for *t*-YS.

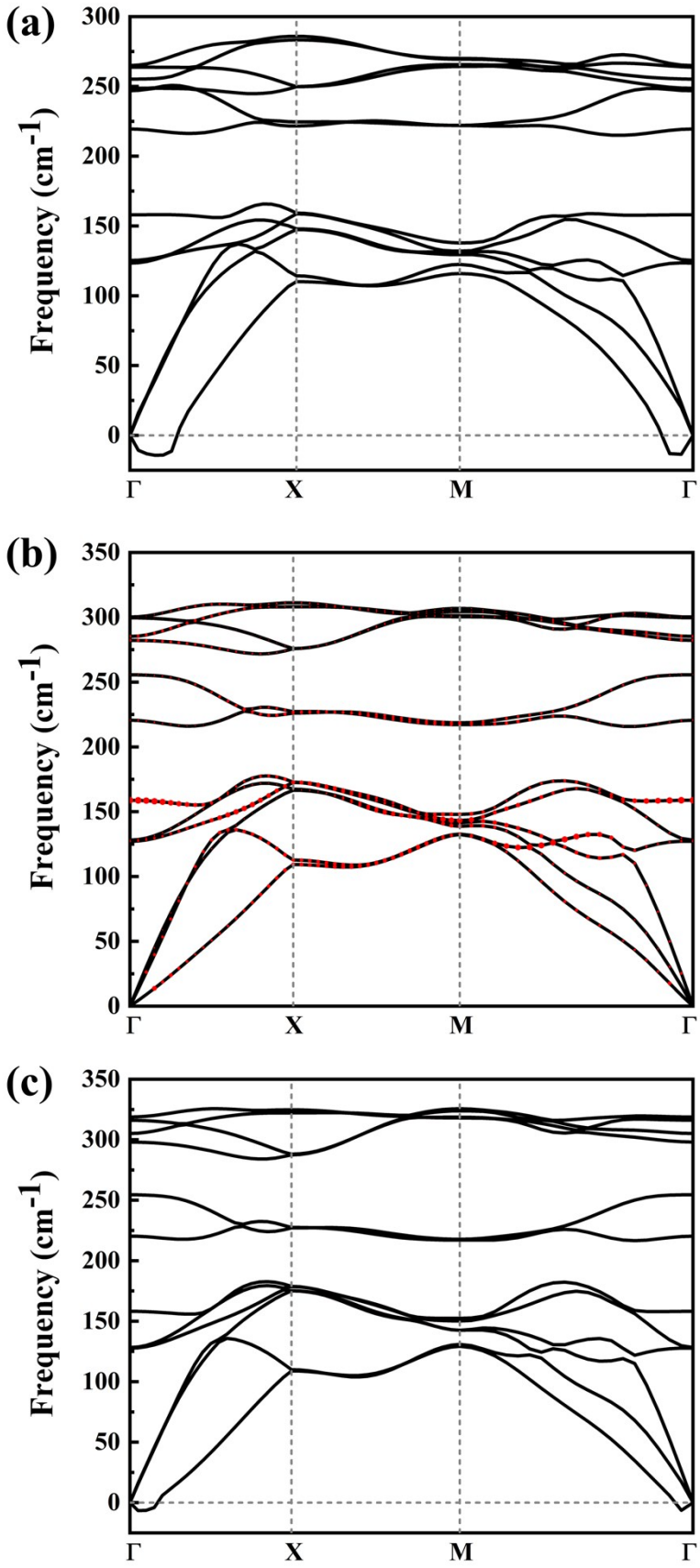

Fig. S6 Phonon frequency dispersions (a) under uniaxial tensile strain of 2%, (b) uniaxial compressive strain of 2% and (c) uniaxial compressive strain of 4% for *t*-YS.

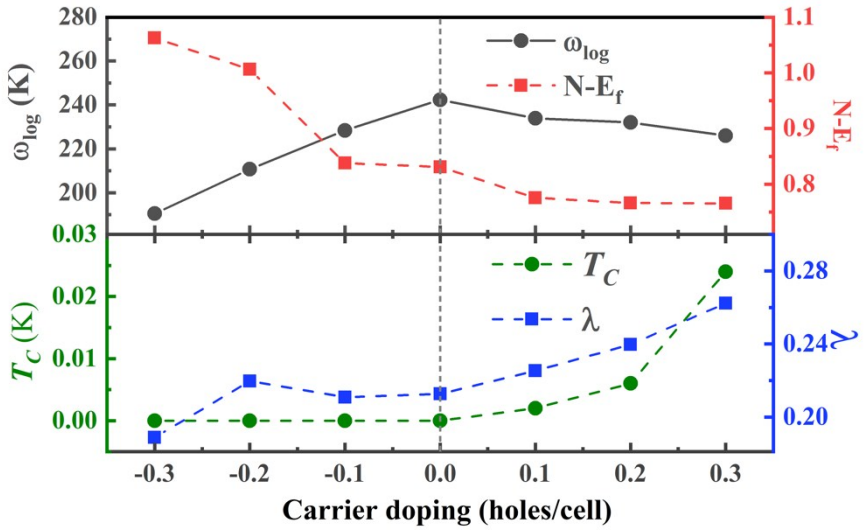

Fig. S7 Doping effects on ω_{log}, N-E_f, T_c and λ of *t*-YS.