Supporting Information

Achieving charge density wave transition at room-temperature in 2D nonlayered transition metal dichalcogenide CoS

Xu He [a, b], *Wenting Hong* [a, b], *Chuanyong Jian* [a, b, c], *Fapeng Sun* [a, b, c], *Qian Cai* [a, b], *and Wei Liu* [a, b *]

[a]CAS Key Laboratory of Design and Assembly of Functional Nanostructures, and Fujian Provincial Key Laboratory of Nanomaterials, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian, 350002, China

[b]Fujian Science & Technology Innovation Laboratory for Optoelectronic Information of China, Fuzhou, Fujian 350108, P. R. China

[c]University of Chinese Academy of Sciences, Beijing, 100049, China

E-mail: liuw@fjirsm.ac.cn

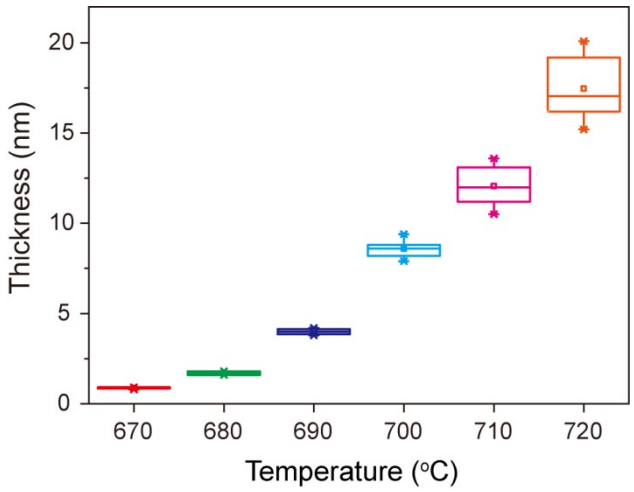

Figure S1. Length statistical box plots of CoS nanoplates grown at different reaction temperatures while keeping all other conditions the same.

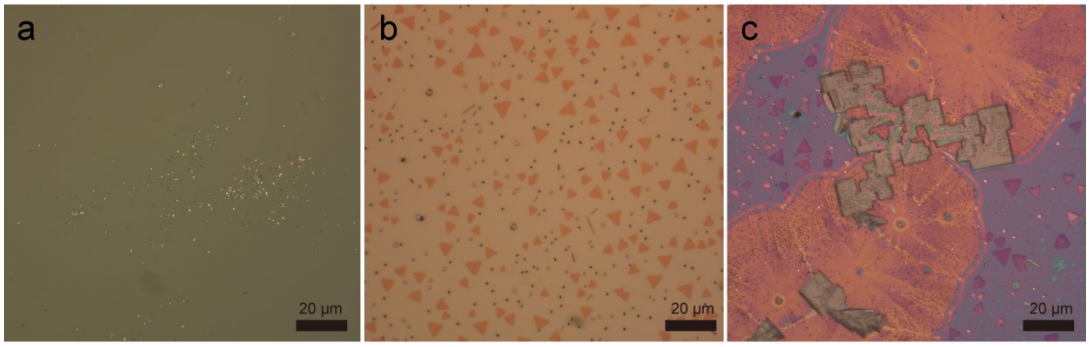

Figure S2. The Optical microscopy images of CoS nanoplates grown with different amounts of NaCl addition. (a) No NaCl. (b) Suitable NaCl (0.002 g). (C) Excess NaCl (0.005 g).

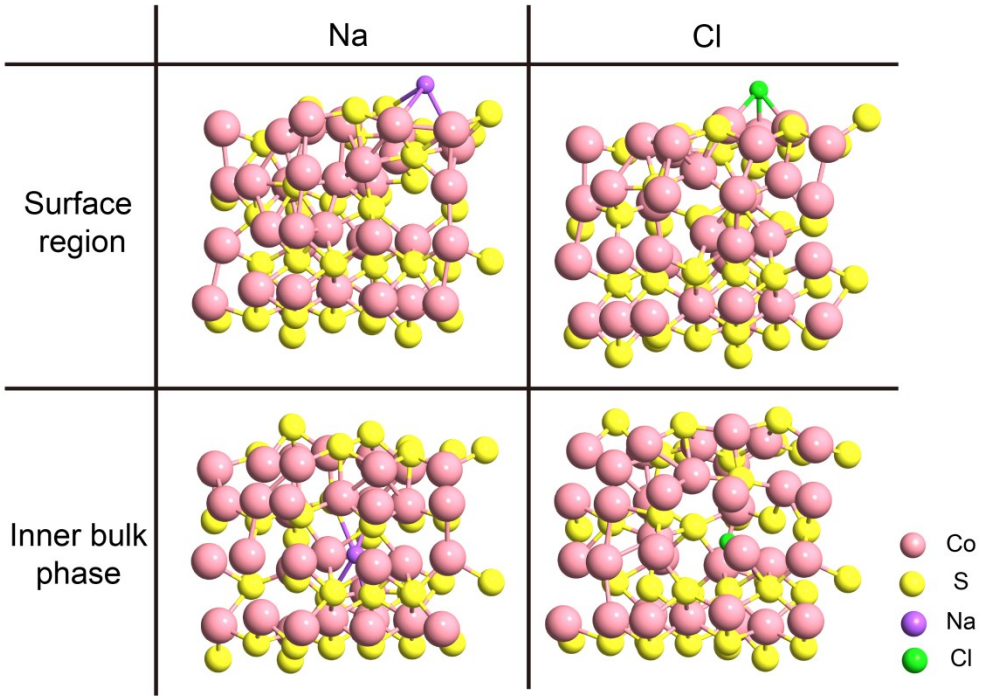

Figure S3. The Density functional theory calculations models of Na or Cl atom adsorb at the CoS (001) plane surface region or inner bulk.

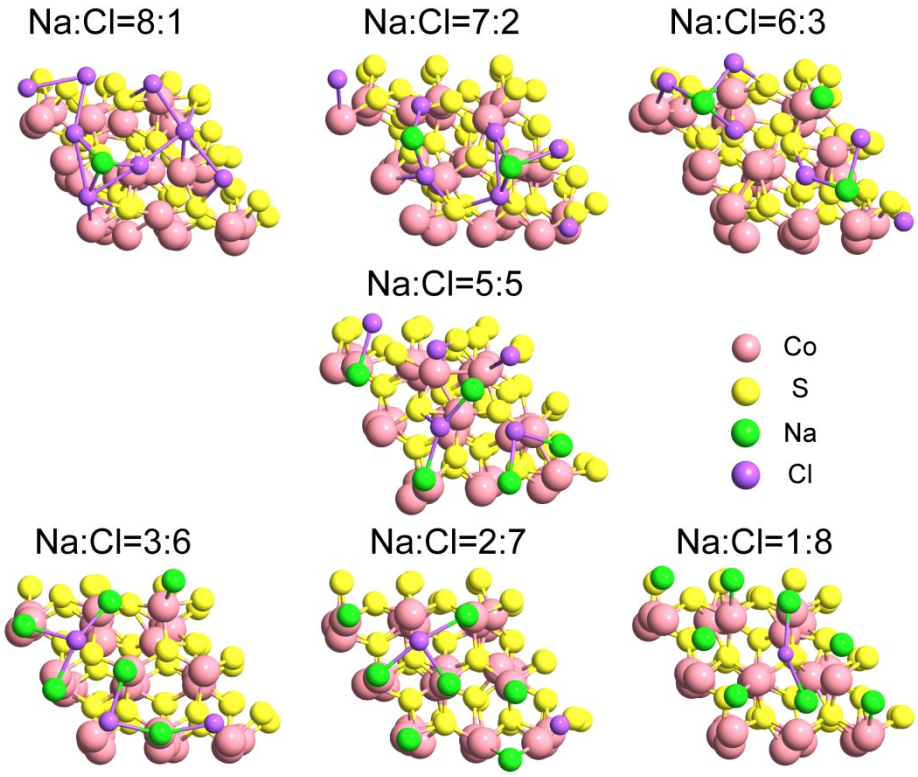

Figure S4. The Density functional theory calculations models of different ratios of Na and Cl adsorb at the (001) plane of the CoS.

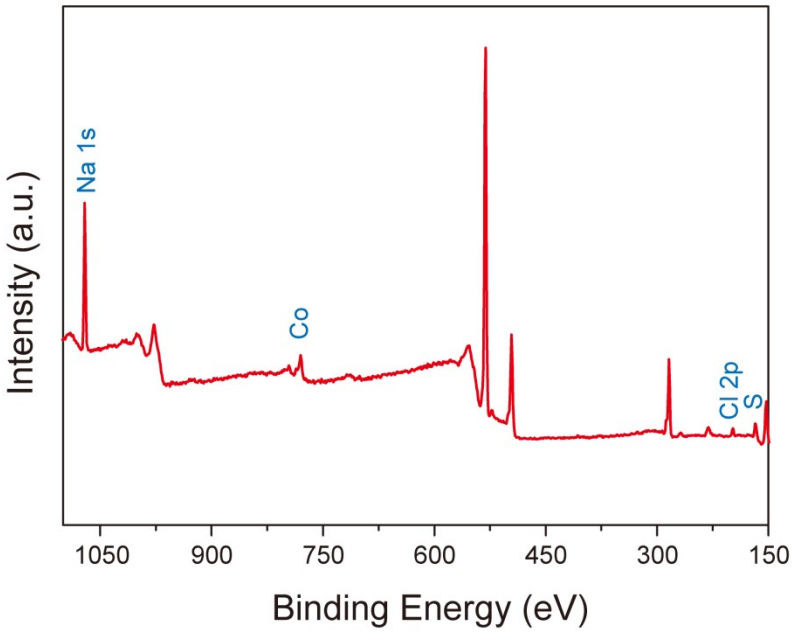

Figure S5. XPS survey spectrum of CoS sample grown on SiO_2/Si substrate, which can show the existence of Na and Cl on the sample substrate to prove Na and Cl absorption growth mechanism.

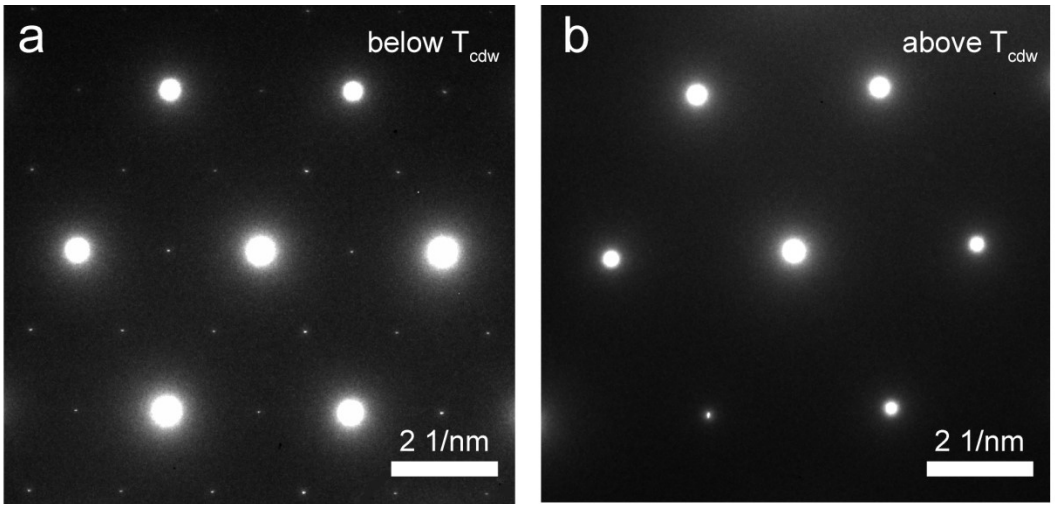

Figure S6. Electron diffraction pattern obtained in a TEM of the CoS single crystal with the measured temperature below (a) and above (b) the CDW phase transition temperature.

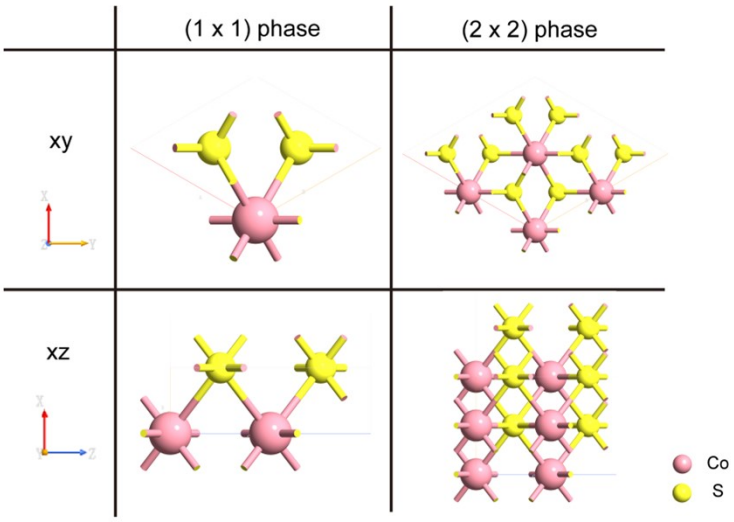

Figure S7. The structural model was used for the simulation of CoS (1 x 1) phase and (2 x 2) phase.

DFT calculation method: All the first-principles spin-polarized calculations are performed using the Vienna ab initio simulation package[1, 2] The ion-electron interactions are described by the hybrid functional HSE06[3] and plane wave cutoff energy of 350 eV for plane-wave basis set were adopted. The electronic iterations convergence is 10^{-5} eV using the Damped molecular dynamics algorithm, and 5×10^{-3} eV/Å for energy and force, respectively, during the structure relaxation. Since the CoS nanoplate has a thickness of few nanometers, the CoS bulk structure models were used to analyze the (1 × 1) normal phase and (2 × 2) CDW phase in the calculation. Based on these conditions, the corresponding (1 × 1) normal phase and (2 × 2) CDW phase for CoS bulk were constructed using the lattice parameter optimized1. The reciprocal space integrations were carried out at the gamma-points. The Brillouin zone integrations are performed using 10×10×6 and 5×5×6 Monkhorst-Pack k-point sampling for (1 × 1) normal phase and (2 × 2) CDW phase, respectively.

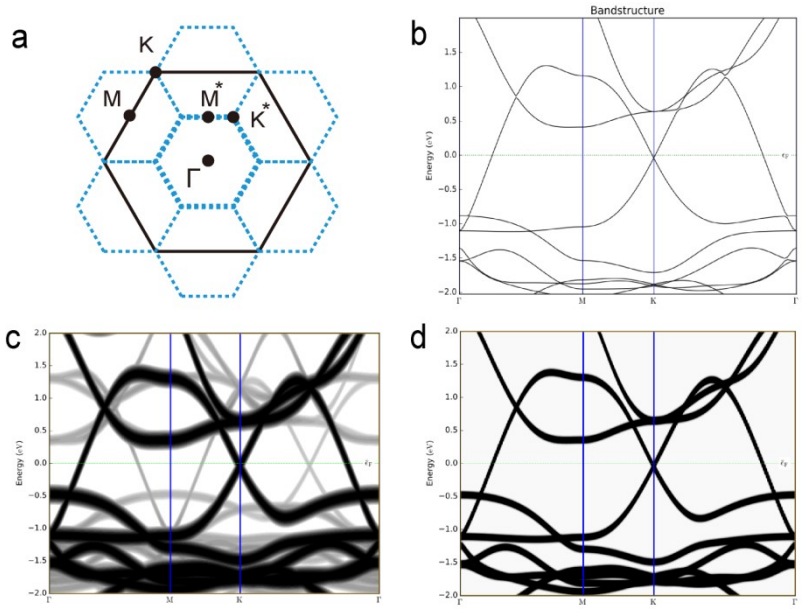

Figure S8. (a) Brillouin zones of the (1 x 1) and (2 x 2) structures outline in black and blue, respectively. (b) Calculated band structure in the (1 x 1) phases. (c) Calculated band structure in the (2 x 2) phases. (d) Calculated band structure of unfold the band structure of the (2 x 2) phase onto the Brillouin zone of the (1 x 1) phase.

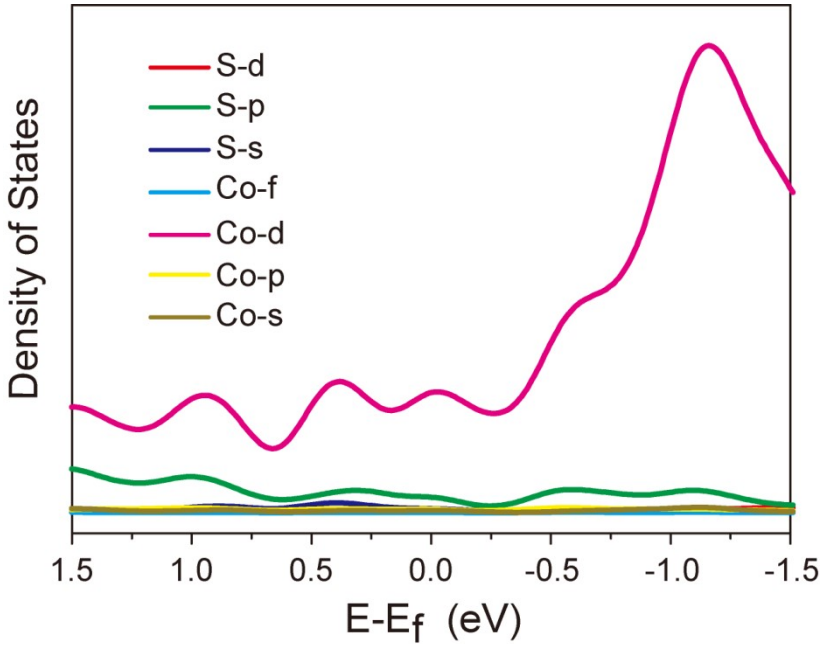

Figure S9. The density of states with different atomic contributions.

Table S1. Comparison of the reported charge density wave (CDW) materials with the highest phase transition temperature.

Material	Control technique	CDW transition temperature range	CDW transition type	Reference
CoS		≈296 K	Metal/Commensurate CDW (CCDW)	This work
$TiTe_2$	Multilayer limit	≈300-673 K	Metal/ CCDW	[4]
1T-$TaSe_2$	pressure	≈190-480 K	Metal/CCDW	[5]
RTe_3	pressure	≈50-416 K	Metal/CCDW	[6]
1T-VSe_2	pressure	≈350 K	Metal/CCDW	[7]
1T-TaS_2	Exfoliation/Gating	≈150-350 K	CCDW/Nearly Commensurate CDW (NCCDW)	[8]
$SmNiC_2$	pressure	≈150-279.3K	Metal/CCDW	[9]
1T-VSe_2	pressure	≈100-240 K	Metal/CCDW	[10]
1T-$TiTe_2$	Pressure quench	≈300K	Metal/CCDW	[11]
2H-$NbSe_2$	Multilayer limit	≈120-150 K	Metal/CCDW	[12]
$TiSe_2$	Thickness	≈187.5-212.5 K	Metal/CCDW	[13]
1T-$TiS_{2-x}Se_x$	Doping	≈150-210 K	CCDW/NCCDW	[14]
K-TaS_2	K intercalation	≈220-300	CCDW/NCCDW	[15]

References

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