Electronic Supplementary Information

Regulating electronic and magnetic properties of 1T'-ReS_2 by fabricating nanoribbons and transition-metal doping: A theoretical study

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Contents:

1. Width and vacuum of zigzag 1T'-ReS_2 nanoribbons.

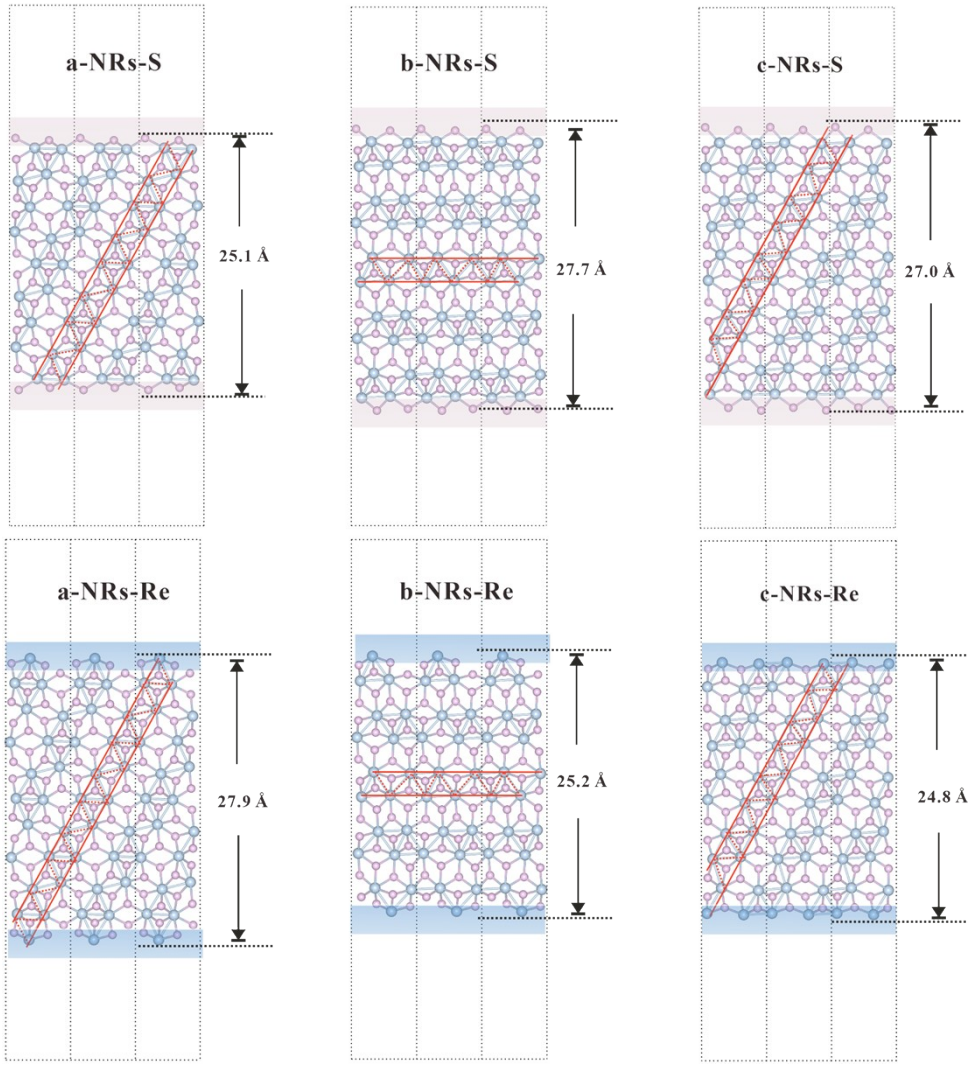

Figure S1 Detailed information of 1T'-ReS_2 nanoribbons (Re, blue ball; S, pink ball) constructed along a, b and c directions shown in Fig. 1a. The diamond-shaped chains consisting with Re4 clusters are also shown with dashed lines to highlight the symmetry features in 1T'-ReS_2 nanoribbons.

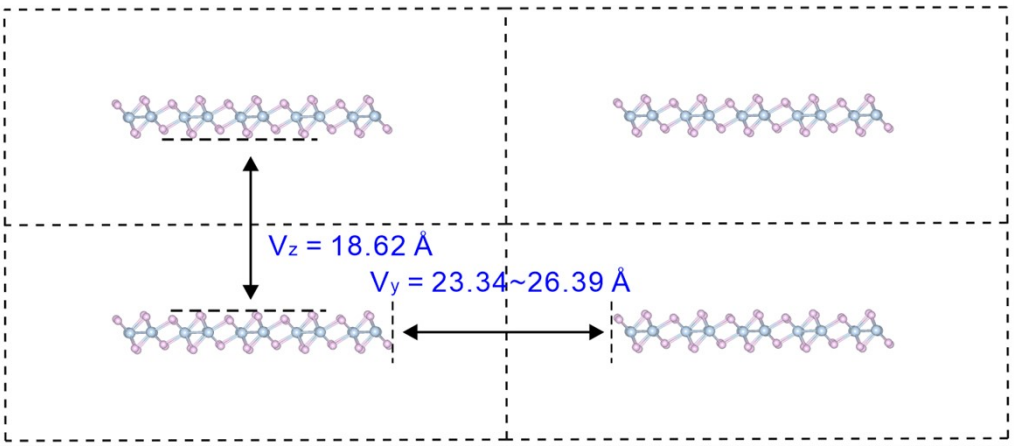

Figure S2 Vacuum of zigzag 1T'-ReS_2NRs (b-NRs-S) along y and z directions.

2. Lattice parameter and the calculated chemical potentials of the transition metals.

Table S1 Lattice parameters and the calculated chemical potentials (μ) of transition metals.

TM*	a/Å	b/Å	c/Å	μ/eV
Cr	2.87	2.87	2.87	-9.65
Mo	2.74	2.74	2.74	-10.85
W	2.76	2.76	2.76	-12.96
Mn	7.46	7.46	7.46	-9.16
Re	**2.79**	**2.79**	**8.97**	**-12.44**
Fe	2.46	2.46	2.46	-8.47
Ru	2.73	2.73	4.31	-9.27
Os	2.76	2.76	4.36	-11.23
Co	2.50	2.50	4.03	-7.11
Rh	2.72	2.72	2.72	-7.36
Ir	2.74	2.74	2.74	-8.84
Ni	2.48	2.48	2.48	-5.78
Pd	2.80	2.80	2.80	-5.18
Pt	2.81	2.81	2.81	-6.07
Cu	2.56	2.56	2.56	-4.10
Ag	2.94	2.94	2.94	-2.83
Au	2.95	2.95	2.95	-3.27

*Note: The lattice parameters of the transition metals are taken from https://materialsproject.org/.

3. Band structures and density of states of monolayer 1T'-ReS_2.

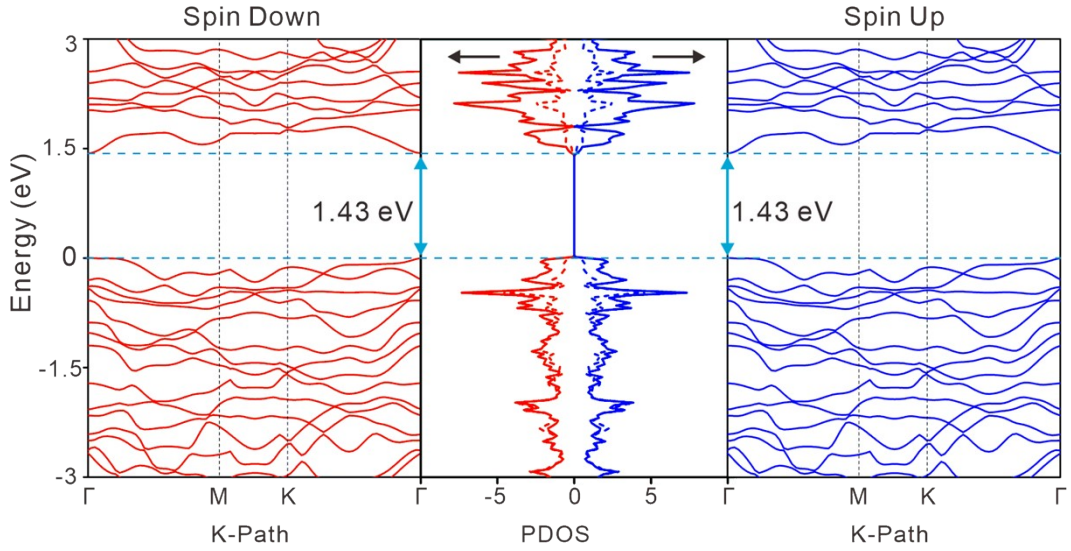

Figure S3 Band structures and density of states of monolayer 1T'-ReS_2. The direct bandgap is also presented for reference. The solid and dashed lines in PDOS represent electron density distributions of Re and S, respectively. Red and blue lines indicate spin down and spin up, respectively.

4. Local structures of a-NRS-S and b-NRS-S before/after doping TM atom of Cr, Mo and Co.

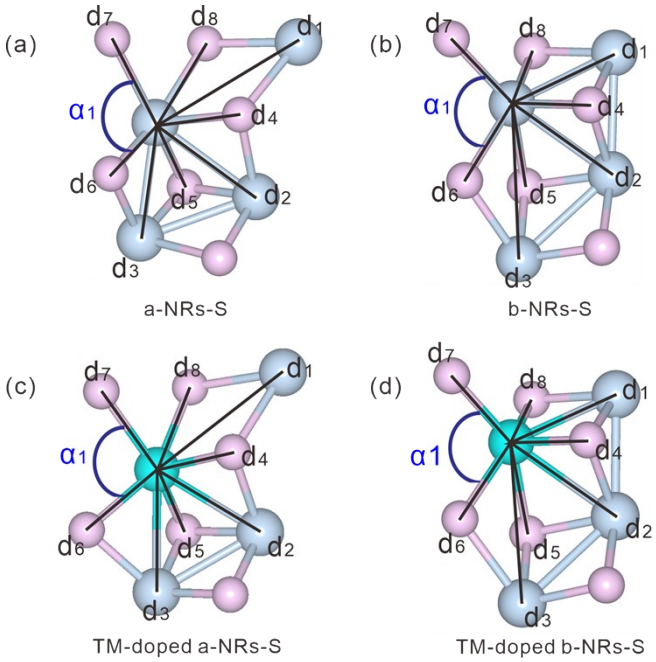

Figure S4 Local structure and parameters describing variations as TM (TM = Cr, Mn, and Co) atom is introduced in a-NRs-S (a) and b-NRs-S (b). The TM atom is highlighted with green in (c) and (d).

Table S2 Nanoribbons, bond lengths and bond angles before/after Cr, Mn and Co are introduced.

Nanoribbons	$\alpha_{1/°}$	d_1/Å	d_2/Å	d_3/Å	d_4/Å	d_5/Å	d_6/Å	d_7/Å	d_8/Å
a-NRs-S	81.14	3.79	2.87	2.68	2.43	2.40	2.47	2.38	2.46
Cr-doped	86.72	3.62	2.73	2.79	2.23	2.26	2.28	2.35	2.40
Mn-doped	86.65	3.58	2.73	2.81	2.27	2.26	2.30	2.32	2.35
Co-doped	86.49	3.56	2.70	2.82	2.22	2.25	2.30	2.22	2.23
b-NRs-S	89.33	2.71	2.83	3.61	2.29	2.43	2.40	2.29	2.36
Cr-doped	90.63	2.66	2.87	3.67	2.22	2.44	2.33	2.20	2.27
Mn-doped	88.78	2.64	2.76	3.62	2.19	2.32	2.29	2.23	2.26
Co-doped	88.35	2.62	2.70	3.56	2.23	2.26	2.30	2.26	2.24

5. The partial density of states contributed by specific elements in 1T'-ReS_2 nanoribbons.

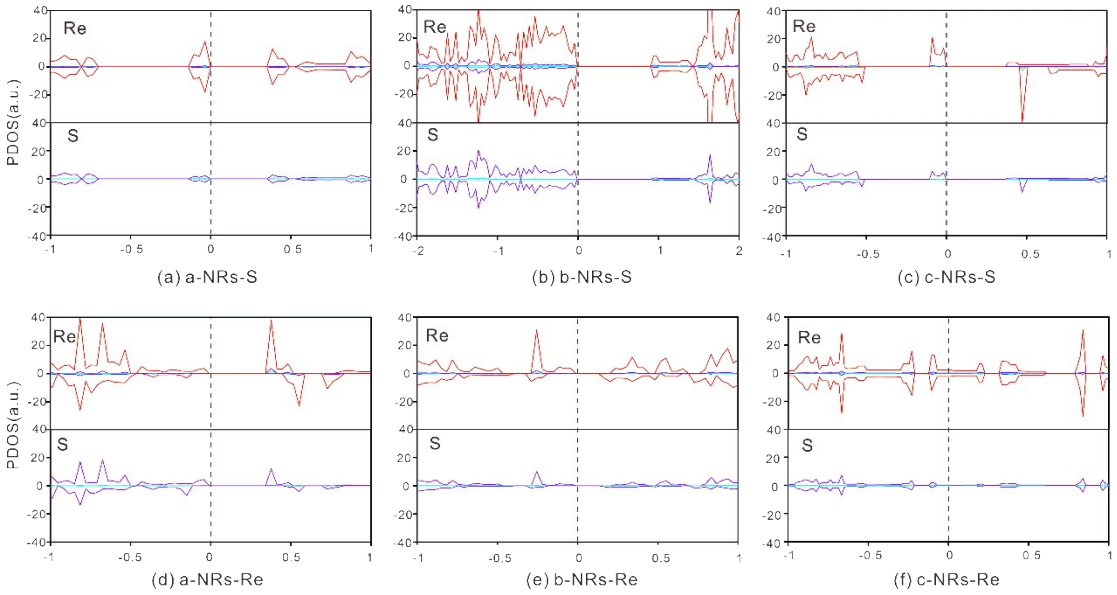

Figure S5 The partial density of states on specific orbitals contributed by composed elements in 1T'-ReS_2 nanoribbons. The lines blue, purple and red represent s, p and d orbitals, respectively.

6. The partial density of states in Mo-, W-, Os-, and Pt-doped a-NRs-S.

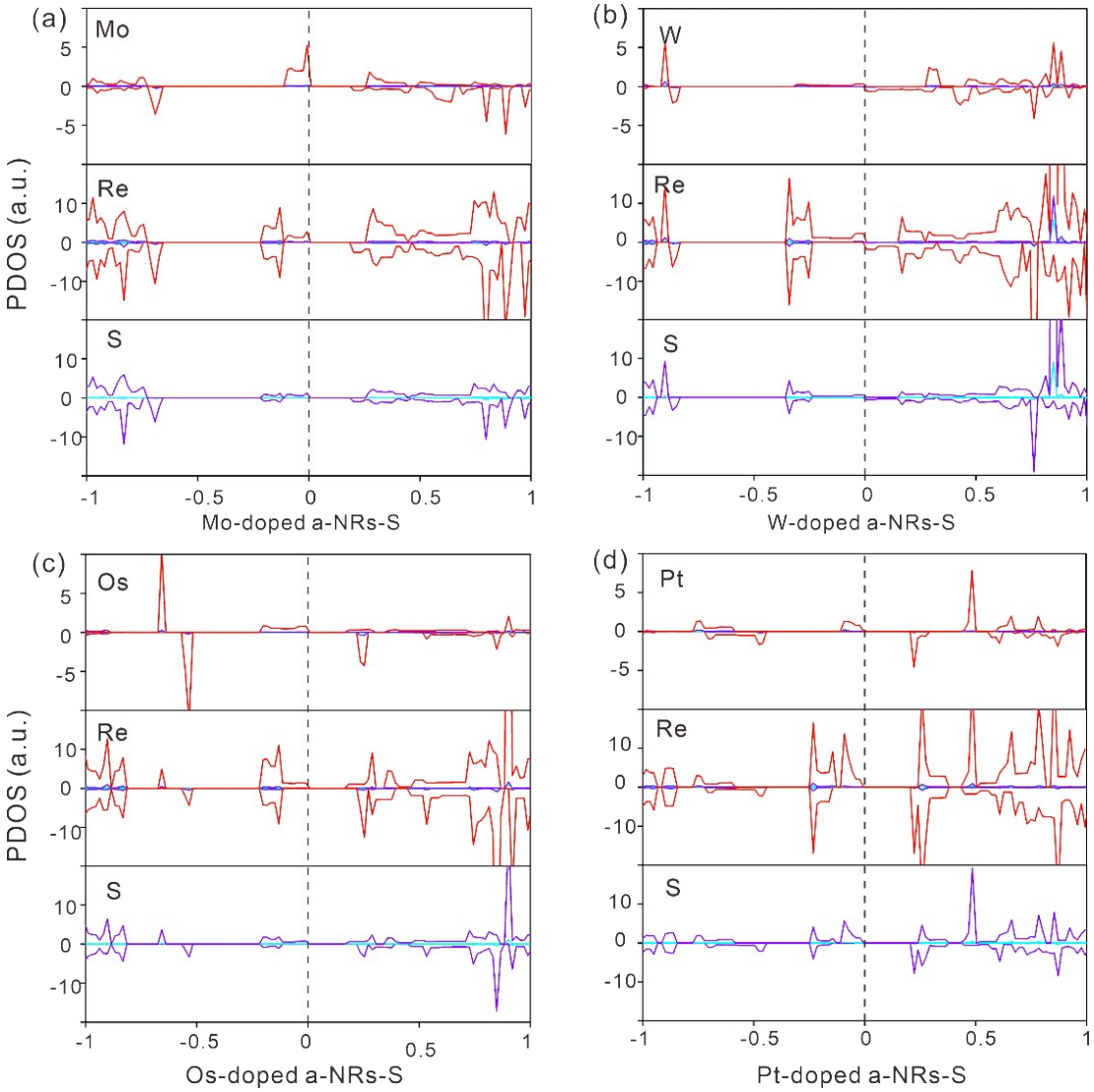

Figure S6 The partial density of states on specific orbitals in Mo-, W-, Os-, and Pt-doped a-NRs-S with magnetism. The asymmetric PDOS distributions indicate magnetism can be introduced in these TM-doped nanoribbons. The lines blue, purple and red represent s, p and d orbitals, respectively.

7. The partial density of states in pristine, Ni-, Pd-, Co-, Rh-, Ir-, Cu-, Ag-, and Au-doped a-NRs-S.

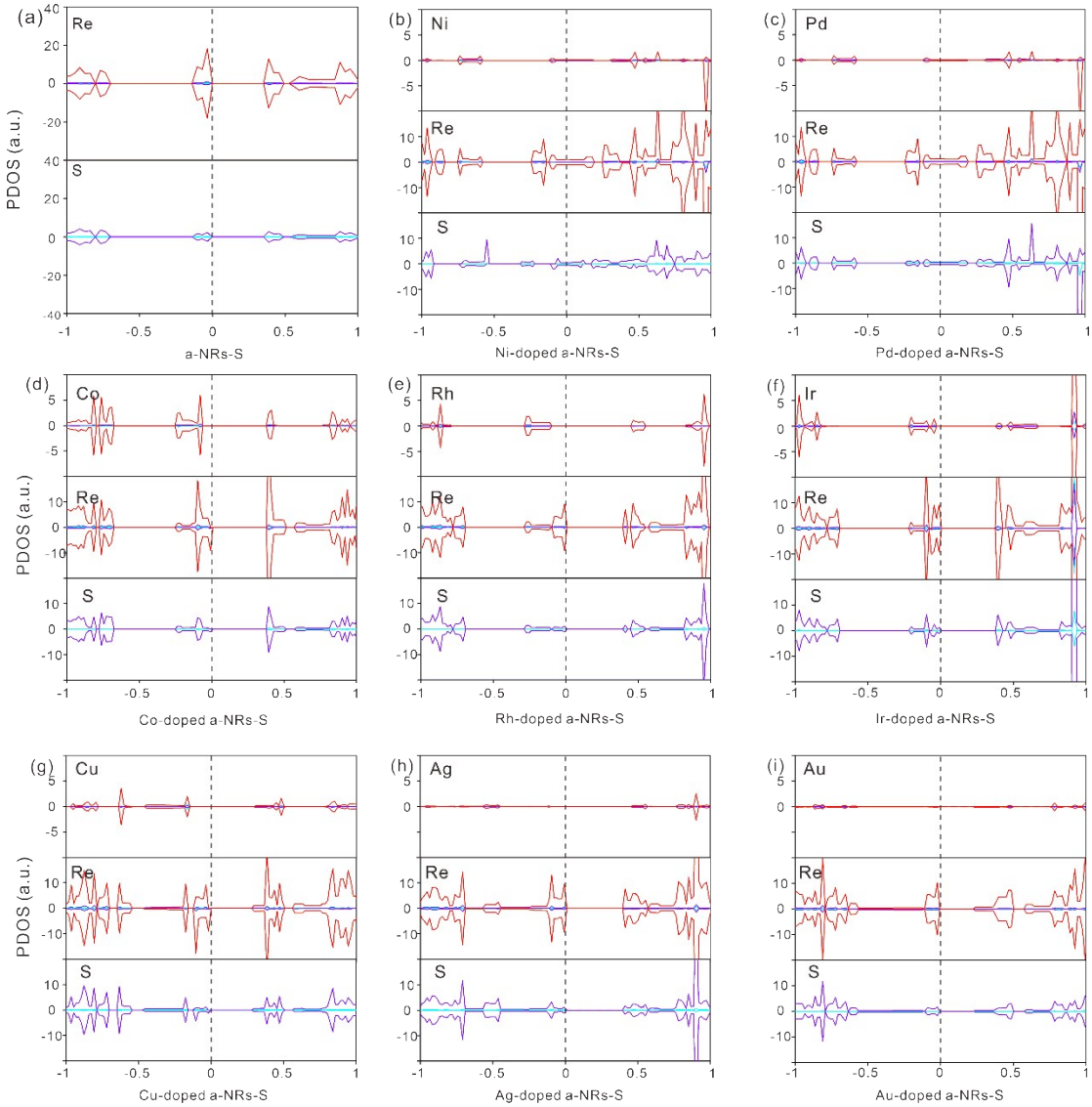

Figure S7 The partial density of states on specific orbitals in pristine, Ni-, Pd-, Co-, Rh-, Ir-, Cu-, Ag-, and Au-doped a-NRs-S. The symmetric PDOS distributions indicate no magnetism exists in these nanoribbons. The lines blue, purple and red represent s, p and d orbitals, respectively.

8. The partial density of states in Cr-, Ni-, Pd- and Pt- doped b-NRs-S.

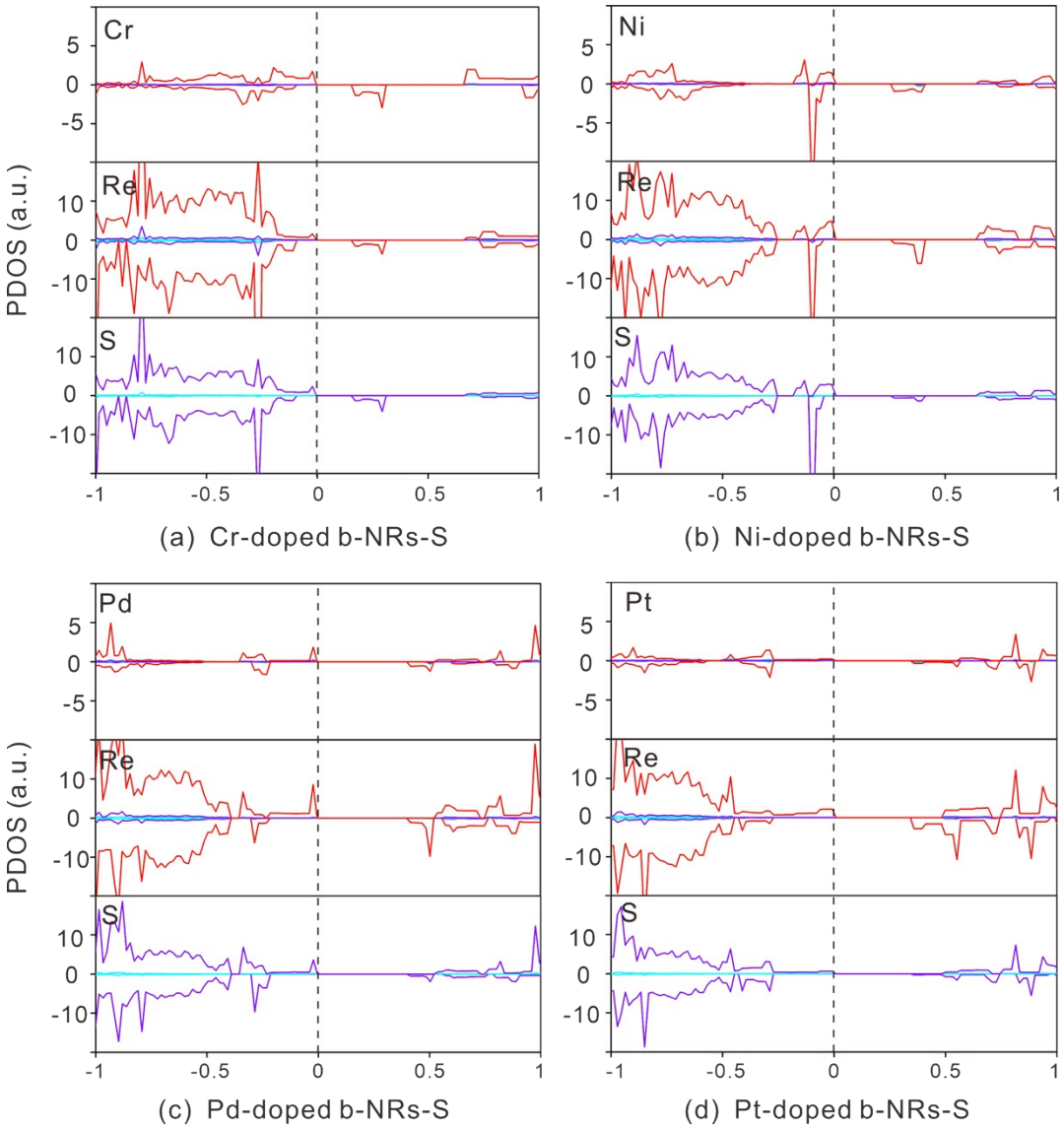

Figure S8 The partial density of states on specific orbitals in Cr-, Ni-, Pd- and Pt- doped b-NRs-S. The asymmetric PDOS distributions indicate magnetism can be introduced by TM-doping in exists in b-NRs-S. The lines blue, purple and red represent s, p and d orbitals, respectively.

9. Bader charge analysis of atoms around doping sites in pristine and TM-doped a-NRs-S nanoribbons.

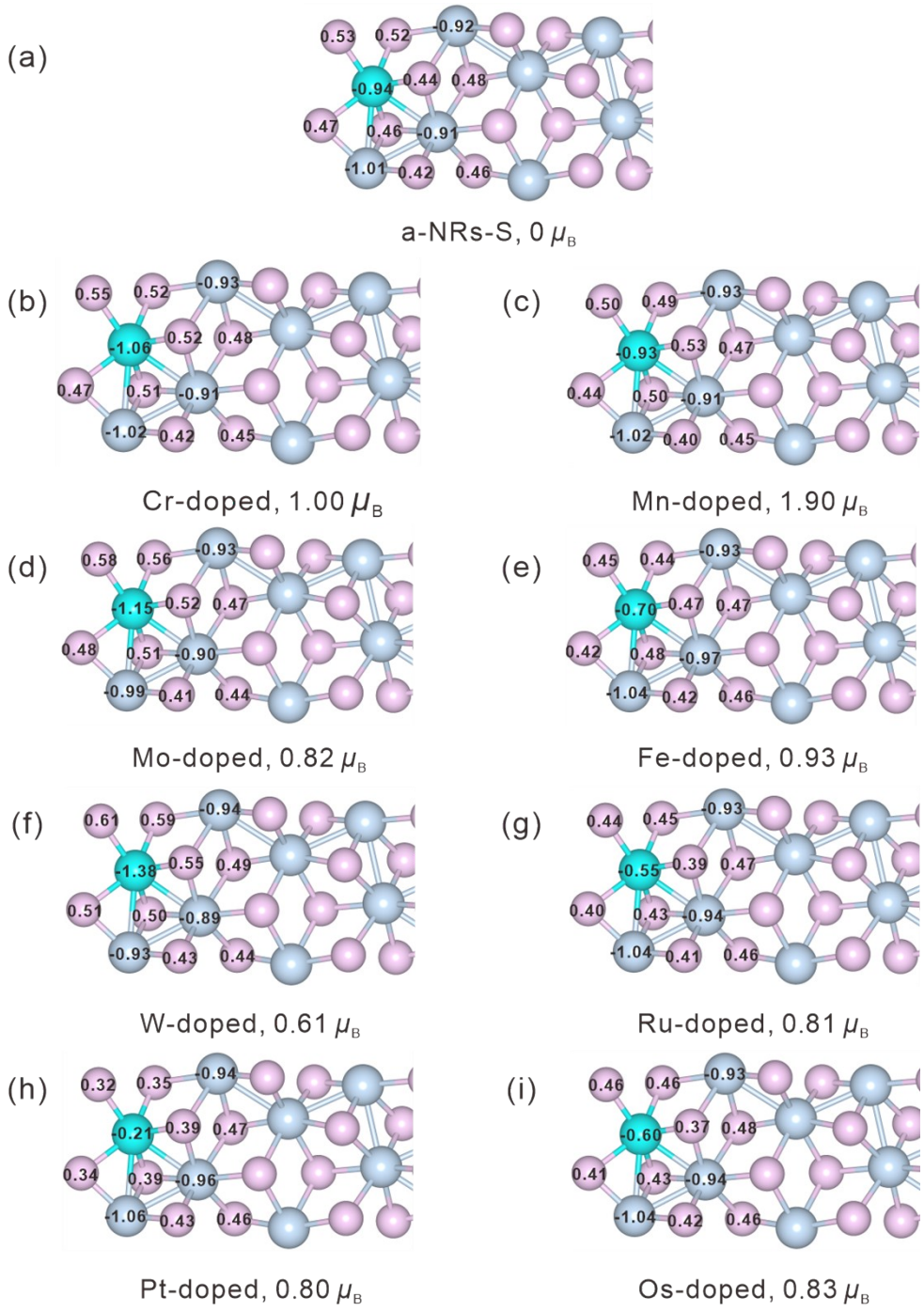

Figure S9 Bader charge analysis of atoms around doping sites in pristine (a) and (b-i) TM-doped a-NRs-S nanoribbons. The detailed Bader charge of TM atom and atoms around it is presented in each panel. Positive and negative values represent accumulation and deletion of electrons, respectively. The total magnetic moment of the nanoribbon is also listed under each panel.