Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

First-principles calculations to investigate strain, electric field, and atom impurities effects on the electronic and magnetic properties of RuX_2 $(X = S, Se)$ nanosheets

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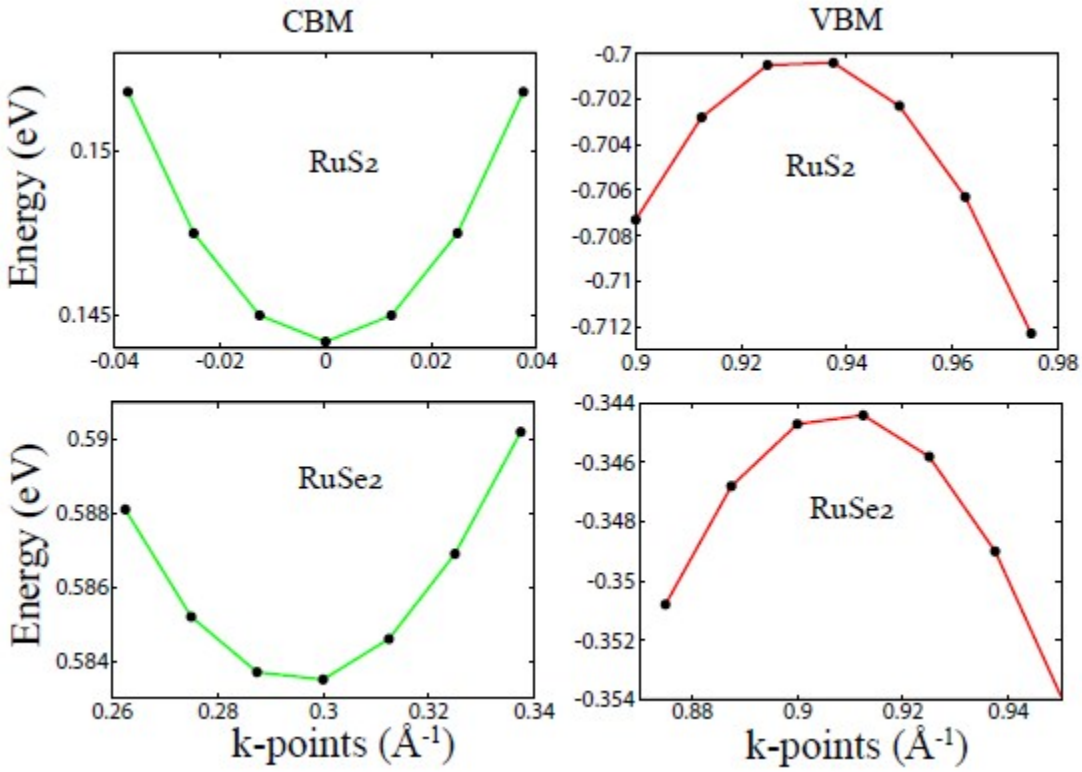

Fig. S1 The E-k points closed to the CBM and VBM plots for $T' - RuX_2$ sheets.

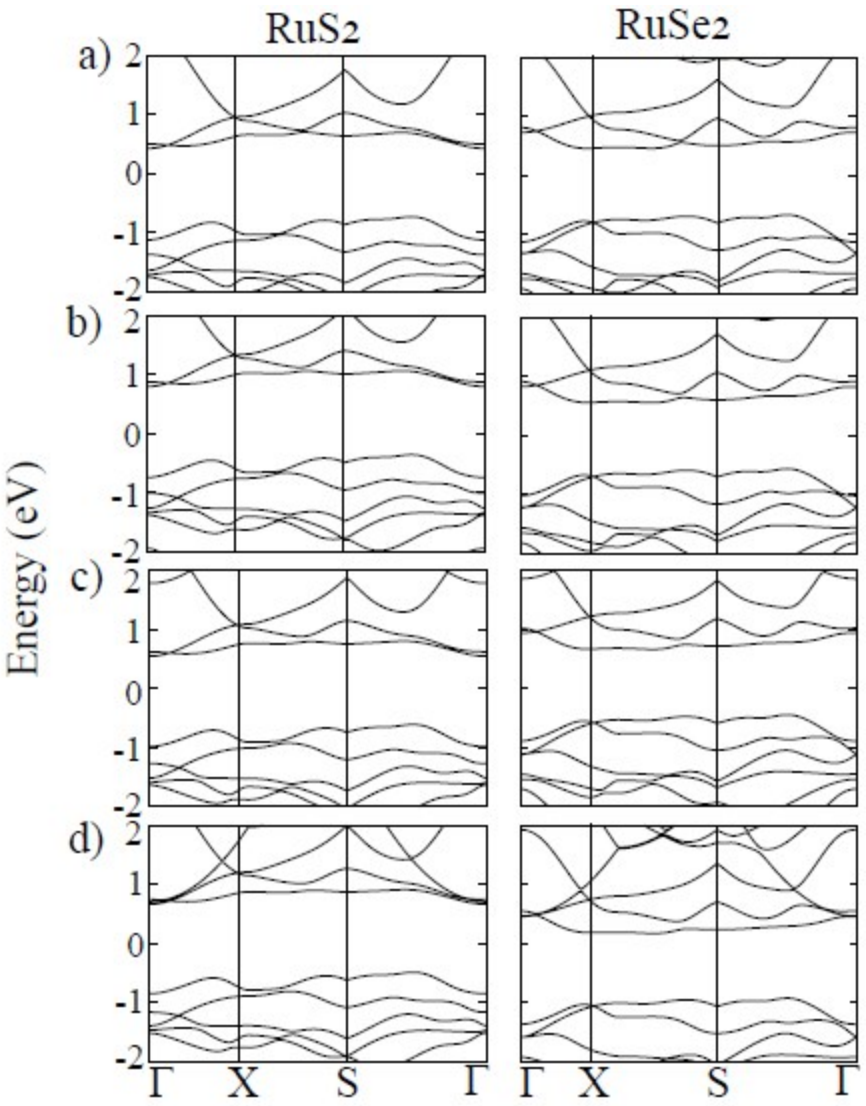

Fig. S2 The band structure for the $T' - RuX_2$ sheets with electric field of magnitude (a) 2 (b) 4 (c) 6 (d) 8 V/nm.

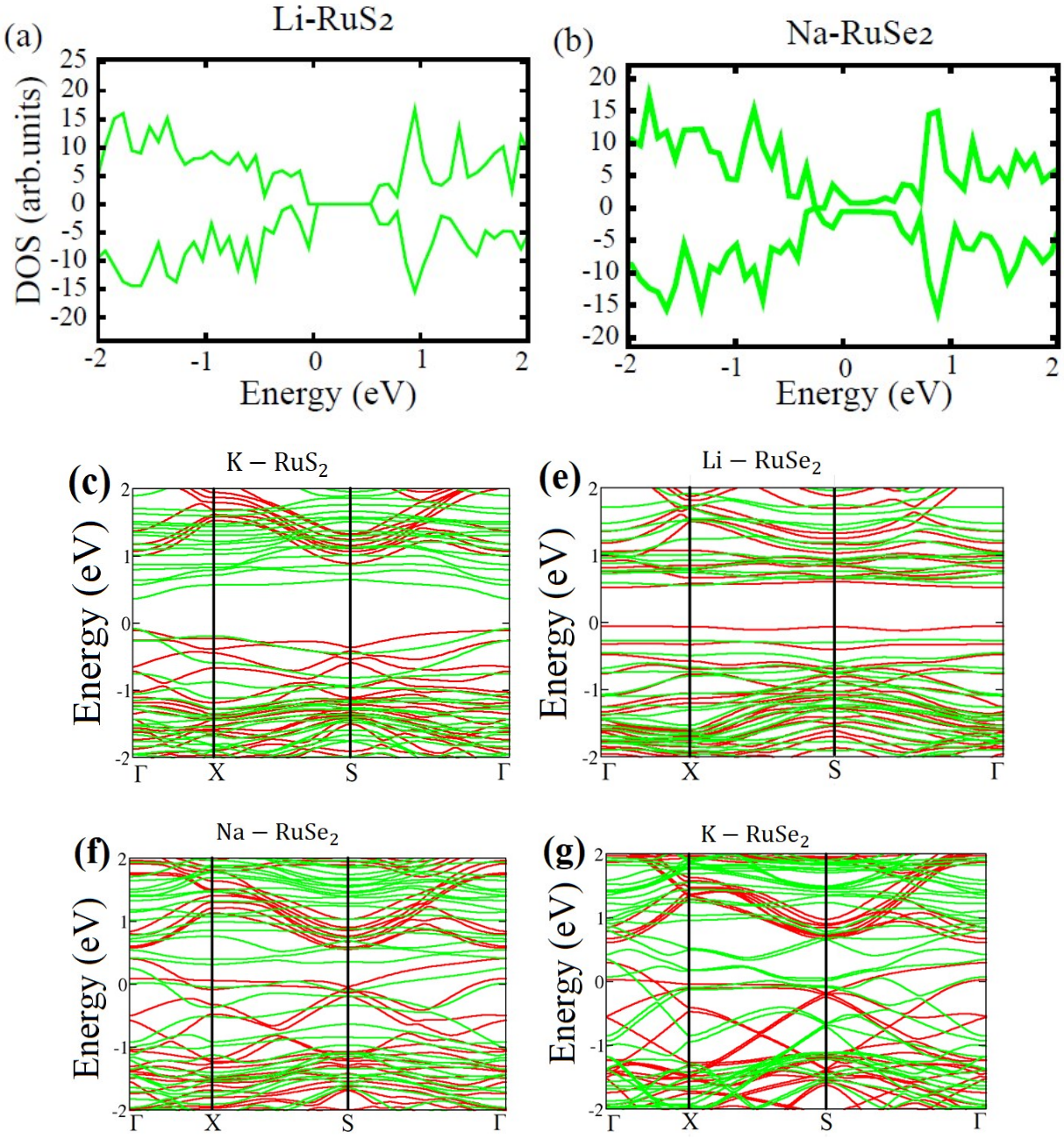

Fig. S3 Spin-polarized DOS and band structures for the (a)-(c) $T^{'} - RuS_2$ (a)-(c) and (d)-(f) $T^{'} - RuSe_2$ with adsorbed Li, Na, K atoms. Red and green color represent spin-up and spin-down bands.

Table S1: The calculated carrier effective mass (m^*) for $T^{'} - RuX_2$ sheets.

Sheet	Carrier	m^*/m_0
RuS_2	e	27.7268
	h	22.4335

$RuSe_2$	e	37.5317
	h	26.5343

Table S2: Relative adsorption energy in eV for Li, Na and K atoms on the T_{Ru}, T_{X1}, T_{X2} $(X = S, Se)$ and T_{bri} adsorption sites (Ads. Site). The adsorption sites are indicated in Fig. 1.

Sheet	Atoms	$E_{T_{Ru}} - E_{T_{X2}}$	$E_{T_{X1}} - E_{T_{X2}}$	$E_{T_{bri}} - E_{T_{X2}}$	Ads. Site
RuS_2	Li	-1.2947	0.0959	0.1955	T_{Ru}
	Na	-0.8963	0.0146	0.0748	T_{Ru}
	K	0.1466	0.4210	0.5569	T_{X2}
$RuSe_2$	Li	-0.0182	0.4199	0.6108	T_{Ru}
	Na	1.6086	0.4887	0.7211	T_{X2}
	K	0.2526	0.7289	0.9286	T_{X2}

Table S3: Relative energies in eV between FM and AFM for $T' - RuX_2$ sheets with adsorbed Li, Na and K atoms.

Sheet	Atoms	$E_{AFM} - E_{FM}$	Magnetic Ordering
RuS_2	Li	-0.0570	AFM
	Na	-0.1771	AFM
	K	0.0535	FM
$RuSe_2$	Li	0.0286	FM
	Na	0.0557	FM
	K	0.1433	FM