Supplementary Material: Electronic and magnetic properties of the monolayer α-$RuCl_3$: A first-principles and Monte Carlo study

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Table I. Calculated relative energy values according to E_{FM} for single layer $RuCl_3$ with and without SOC in meV/atom.

	FM	NM	Neel	Stripy	Zigzag
E_{rel}	0	25.6	20.0	8.1	6.9
E_{rel}^{SOC}	0	20.6	18.1	6.3	5.0

Table II. Calculated exchange interaction parameters J_1, J_2, J_3 for single layer $RuCl_3$ with and without SOC.

	J_1 (meV)	J_2 (meV)	J_3 (meV)
w/o SOC	10.69	−1.26	2.54
w/ SOC	9.71	−1.59	2.19

Table III. Magneto-crystalline anisotropy energies for FM configuration of single $RuCl_3$ using GGA+SOC

out of plane
$E[100] - E[001] = -18.88\ meV$
in-plane
$E[100] - E[010] = 61\ \mu eV$

Table IV. Orbital magnetic moment per Ru atom (μ_B/atom) in single layer $RuCl_3$ for different magnetization directions

	[001]	[010]	[100]	[110]	[011]	[101]	[111]
μ_l	0.833	0.825	0.825	0.825	0.829	0.828	0.827

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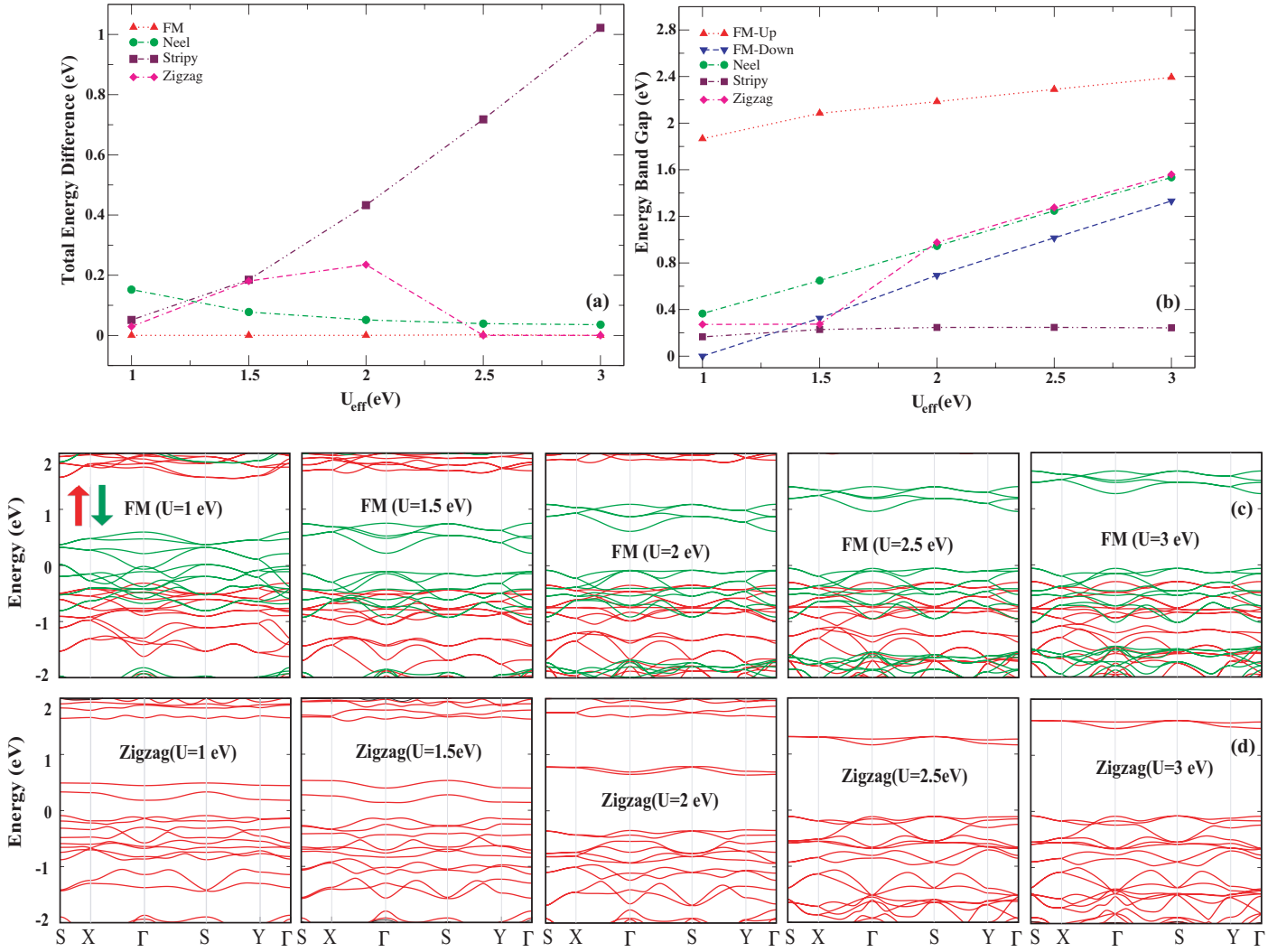

Figure 1. (Color online)(a) Relative energy difference for each configuration with respect to U_{eff}. (b) Calculated energy band gap values of all magnetic configurations as a function of U_{eff}. (c)-(d) The effect of on-site Coulomb interaction on the electronic structure of single layer $RuCl_3$ in FM and Zigzag magnetic order, respectively.