Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Searching for active binary rutile oxide catalyst for water splitting from first principles

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Table S1. The differential adsorption energy of O atom (δG(O)) for $RuNiO_2$ and $RuCoO_2$ from DFT and DFT+U calculations (Unit: eV)

	$RuNiO_2$		$RuCoO_2$	
	DFT	DFT+U	DFT	DFT+U
1/3MLO	-0.29	-0.33	-0.68	-0.65
2/3MLO	-0.42	-0.50	-0.58	-0.58
1MLO	-0.48	-0.39	-0.50	-0.47
4/3MLO	0.28	0.25	0.44	0.44

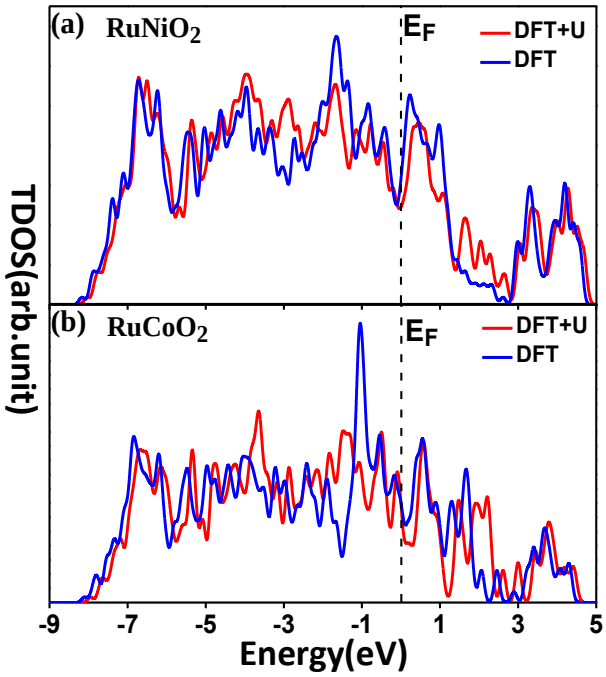

Figure S1. Total density of states of (a) $RuNiO_2$ and (b) $RuCoO_2$ from DFT and DFT+U calculations.