A first principles study on vacancy-defected and transition metal-doped novel Ga_2O_2 monolayers

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We investigate the structural, electronic, and magnetic characteristics of the newly theorized two-dimensional (2D) Ga_2O_2 monolayer [1], considering the influence of vacancy defects and transition metal (TM) doping using first principles calculations. Formation energy calculations suggest the experimental viability of most of the considered structures and doping scenarios, with the exceptions of Ga vacancies and Mn doping. Our findings reveal that the majority of transition metals, excluding Sc, Ti, and Cu, are capable of inducing magnetic properties within the monolayer. Importantly, V and Ti doping leads to a significant n-type conductivity in the typically p-type Ga_2O_2 monolayer. Consequently, TM doping and substitution offer a promising route to introduce n-type behavior and magnetism into the inherently p-type, non-magnetic Ga_2O_2 monolayer.

References

[1] Li Shao, et. al., Phys. Chem. Chem. Phys., 2021,23, 666-673

Figures

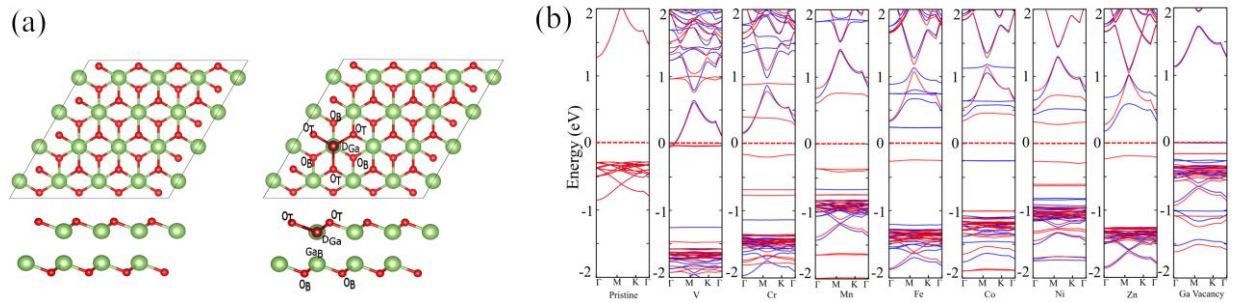

Figure 1: (a)Schematic structures of pristine and defected Ga_2O_2 monolayer. Green and red balls correspond to Ga and O atoms. Top panel: Top view, Bottom panel: Side view, Left panel: Pristine Ga_2O_2 monolayer, Right panel: Defected Ga_2O_2 monolayer (b) Spin resolved band structures of pristine and, defected 2D Ga_2O_2 monolayer for cases demonstrating magnetic moments (V, Cr, Mn, Fe, Co, Ni, Zn doping and, Ga vacancy). The red and blue lines represent the up-spin and down-spin bands.

(a)

System	$E_g(eV)$	M_{tot} (M_{defect})	E_{form}(eV)	
			Ga Rich	O Rich
Pristine	1.56	-	-	-
Ga Vacancy	metal	1(-)	3.41	0.53
O Vacancy	1.41	-	-4.91	-2.03
Sc	1.06	-	-1.94	-4.82
Ti	metal	-	-0.32	-3.20
V	metal	2(1.63)	-0.25	-2.62
Cr	0.33	3(2.67)	1.28	-1.60
Mn	0.95	4(3.75)	3.12	0.25
Fe	0.45	5(3.69)	1.75	-1.13
Co	0.56	2(1.95)	2.65	-0.23
Ni	0.60	1(0.97)	2.62	-0.26
Cu	0.08	-	2.10	-0.26
Zn	0.36	1(0.01)	-2.21	-5.09

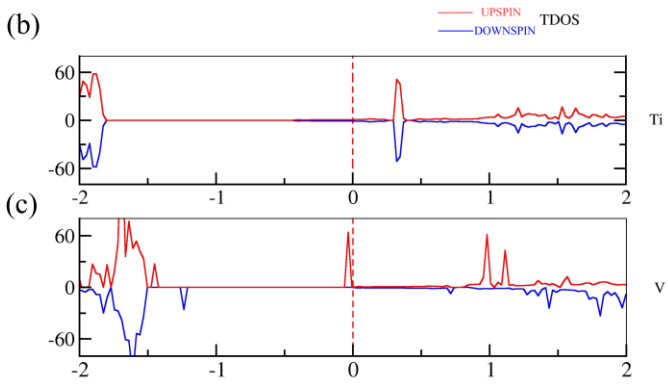

Figure 2: (a) Table demonstrating band gap (E_g), total magnetic moment M_{Tot} and magnetic moment at the defect site (M_{defect}) and, formation energy (E_{form}) of the pristine and defected Ga_2O_2 monolayer; (b) DOS of the Ti doped Ga_2O_2 monolayer demonstrating non-magnetic n-type nature, (c) DOS of the V doped Ga_2O_2 monolayer demonstrating magnetic n-type nature.