Electronic Supplementary Material (ESI) for Nanoscale.

Supporting information

Theoretical Screening of Single Atom Doping on β-Ga_2O_3 (100) for Photoelectrochemical Water Splitting with High Activity and Low Limiting Potential

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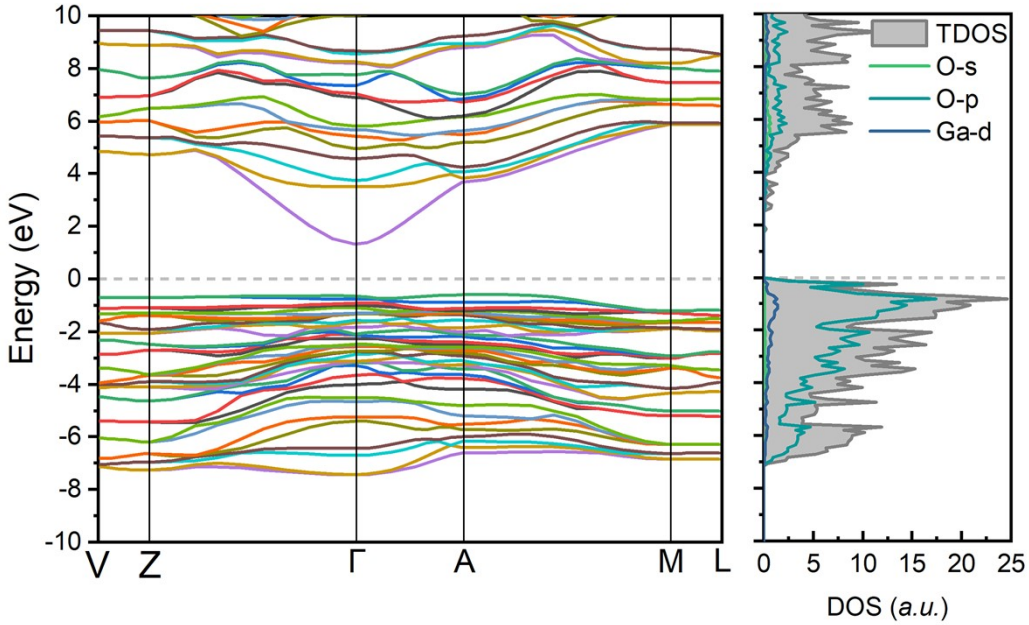

Figure S1 GGA band structure, TDOS and POS analysis of β-Ga_2O_3 unit cell. The top of the valence band is aligned to zero.

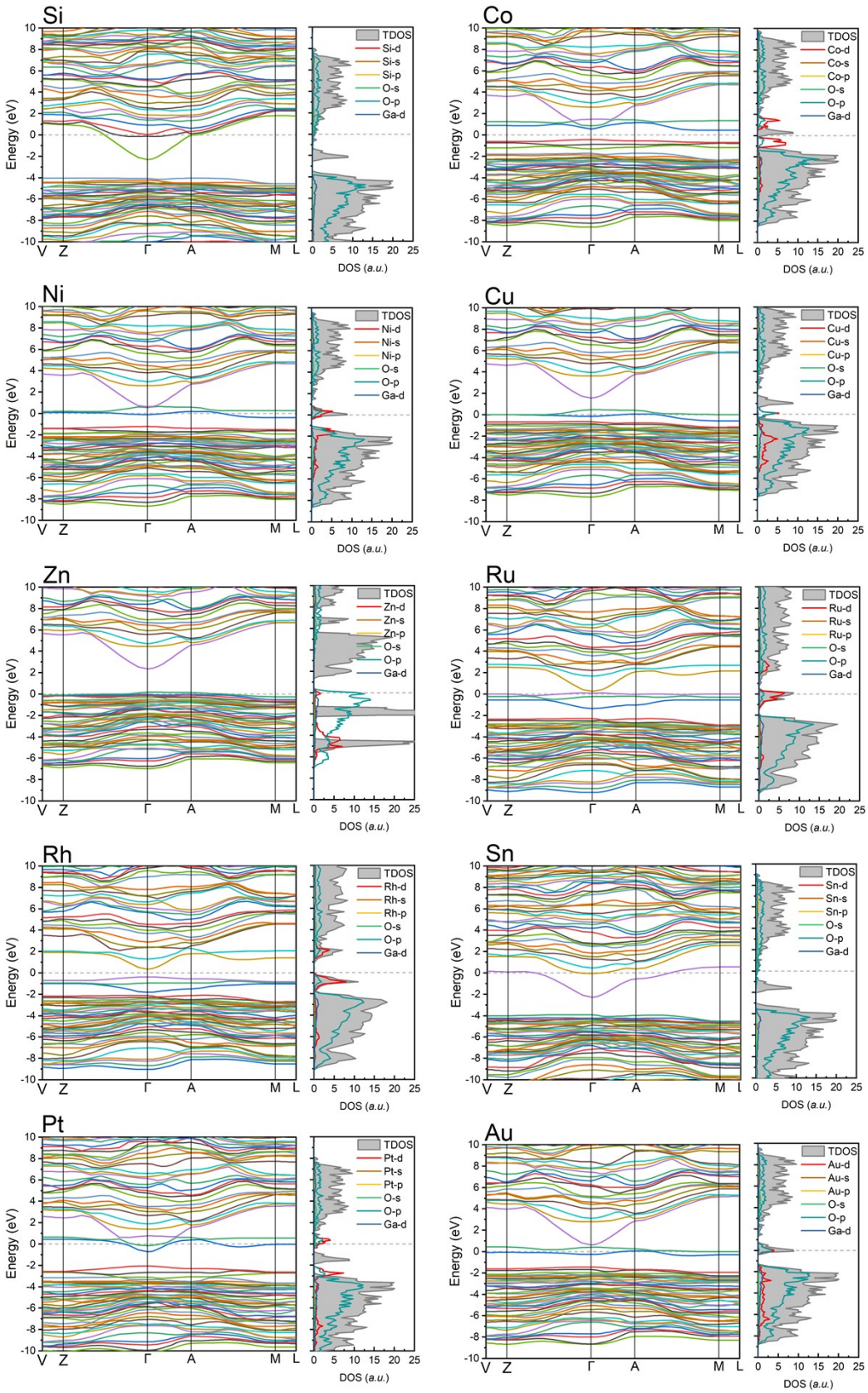

Figure S2 GGA band structure and TDOS and POS analysis of all doped structures.

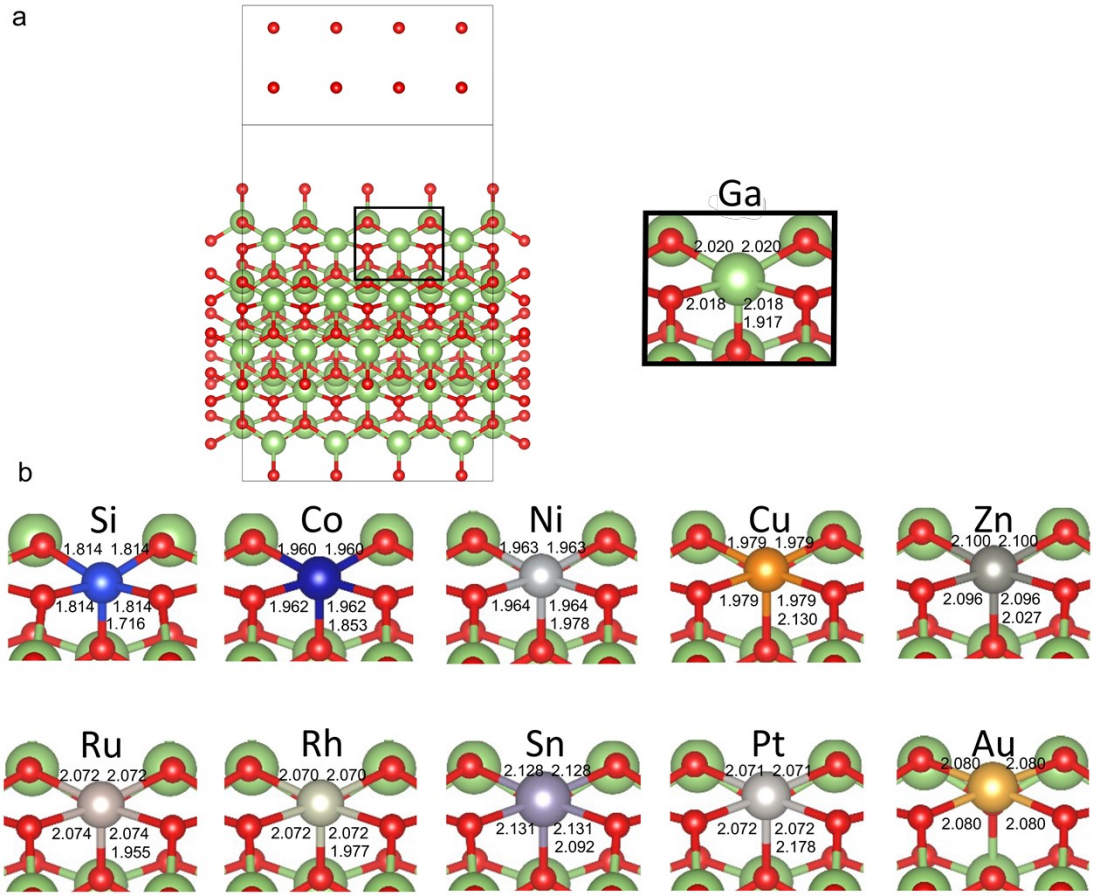

Figure S3 (a) Schematic representation of (100) β-Ga_2O_3 surface. Colour code: Ga, green; O, red. The local structure of Ga is shown in the black box with the bond length. (b) The local structures of other doped structures.

Table S1 Summary of the studied on doped gallium oxide materials.

Year	Material	Method	Research aspect	ref
2012	Zn doped β-Ga_2O_3	Computation	Electronic structures, and absorption and reflectivity in the UV region	[1]
2012	Zn doped Ga_2O_3	Experiment	The effect of different Zn doping concentration in photocatalytic hydrogen production	[2]
2012	Zn doped β-Ga_2O_3 films	Experiment	The microstructure, optical transmittance, optical absorption, optical energy gap, and photoluminescence	[3]
2013	Si doped β-Ga_2O_3	Experiment	Application in fabrication of low-resistance ohmic contacts	[4]
2013	1D nanoporous Zn doped Ga_2O_3	Experiment	Application in photocatalytic hydrogen production	[5]
2013	Zn and Pb	Experiment	Application in photocatalytic hydrogen production	[6]
2015	Non-metal doping	Computation	The photocatalytic redox ability for doped systems	[7]
2017	Al doped β-Ga_2O_3	Computation	The effects of intrinsic defects on electronic structures and optical properties	[8]
2017	Ca/La/Ti doped β-Ga_2O_3	Computation	Geometrical structures and electronic properties	[9]
2018	Rh doped β-Ga_2O_3	Experiment	Application in photocatalytic CO_2 reduction	[10]
2019	N doped β-Ga_2O_3	Computation	The effects of the doping concentration on the electronic and optical properties	[11]
2021	Sr doped β-Ga_2O_3	Computation	The effect of Sr doping in Ga_2O_3 as p-type doping based on its material properties in the simulation structure	[12]
2021	Al doped β-Ga_2O_3 nanostructure	Experiment	The effects of Al doping on hydrothermal synthesized β-Ga_2O_3 nanostructures for photocatalyst applications	[13]
2021	Zn and Ca doped β-Ga_2O_3	Experiment	The effects of core-shell double doping on enhancing photocatalytic activity for hydrogen production	[14]

Table S2 The free energies of the most stable configurations for all the adsorbents on doping structures and pure β-Ga_2O_3 100 surface.

	Slab (eV)	*OH (eV)	*O (eV)	*OOH (eV)
Si	-975.25	-986.68	-980.24	-990.68
Co	-972.89	-983.01	-977.26	-987.71
Ni	-970.96	-980.94	-974.67	-985.70
Cu	-968.59	-977.52	-971.16	-982.51
Zn	-967.47	-975.79	-969.17	-980.94
Ru	-974.56	-985.94	-981.63	-990.76
Rh-Ga1	-972.89	-983.60	-978.20	-988.22
Rh-Ga2	-970.93	-981.97	-976.37	-986.14
Sn	-971.80	-983.39	-976.61	-987.38
Pt	-970.81	-982.11	-976.16	-986.33
Au	-967.66	-976.79	-970.92	-980.91
Ga	-971.91	-982.53	-974.01	-985.56

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