Supplementary Information

Theoretical design of active Ga_2O_3 monolayer-based catalysts for electrocatalytic HER

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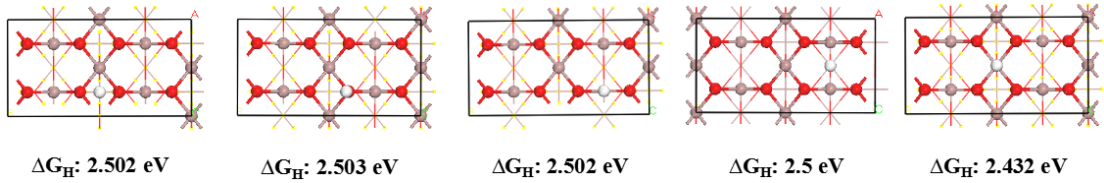

Fig. S1 The top views of H adsorption structures of Ga_2O_3 monolayer, the corresponding H adsorption free energies are listed below the structures. The gray, red and white balls represent Ga, O and H atoms, respectively.

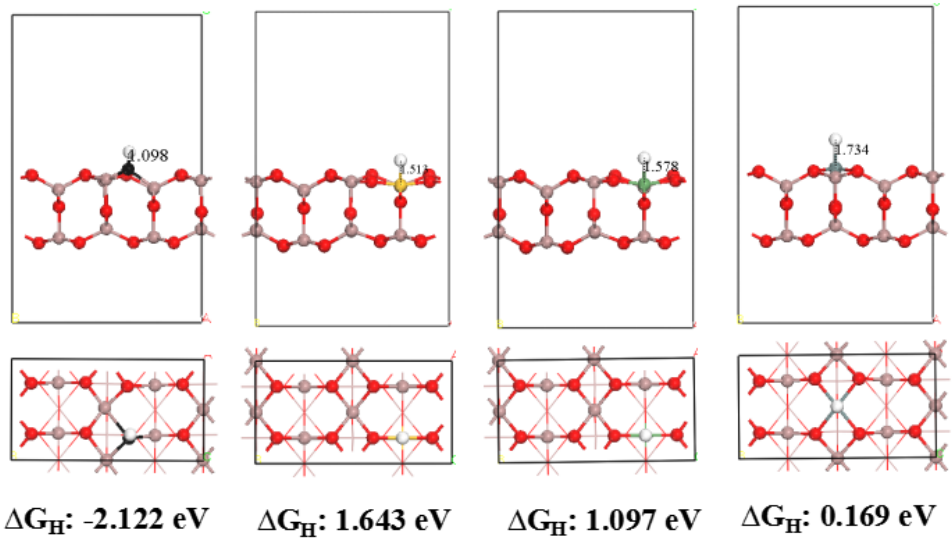

Fig. S2 Top-views and side-views of H adsorption structures of group IV_A elements doped Ga_2O_3 monolayers, the corresponding ΔG_H are listed below the structures. The black, yellow, green and blue balls represent C, Si, Ge and Sn atoms, respectively.

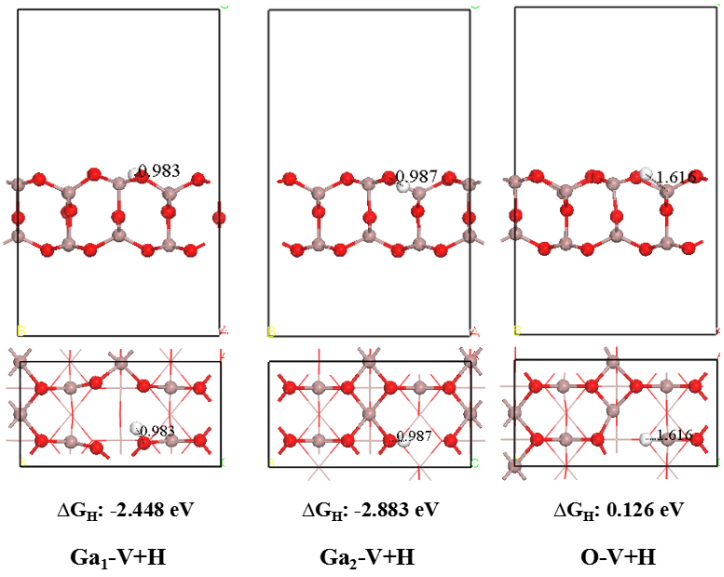

Fig. S3 Top-views and side-views of H adsorption structures of various defected Ga_2O_3 monolayers, the corresponding ΔG_H are listed below the structures.

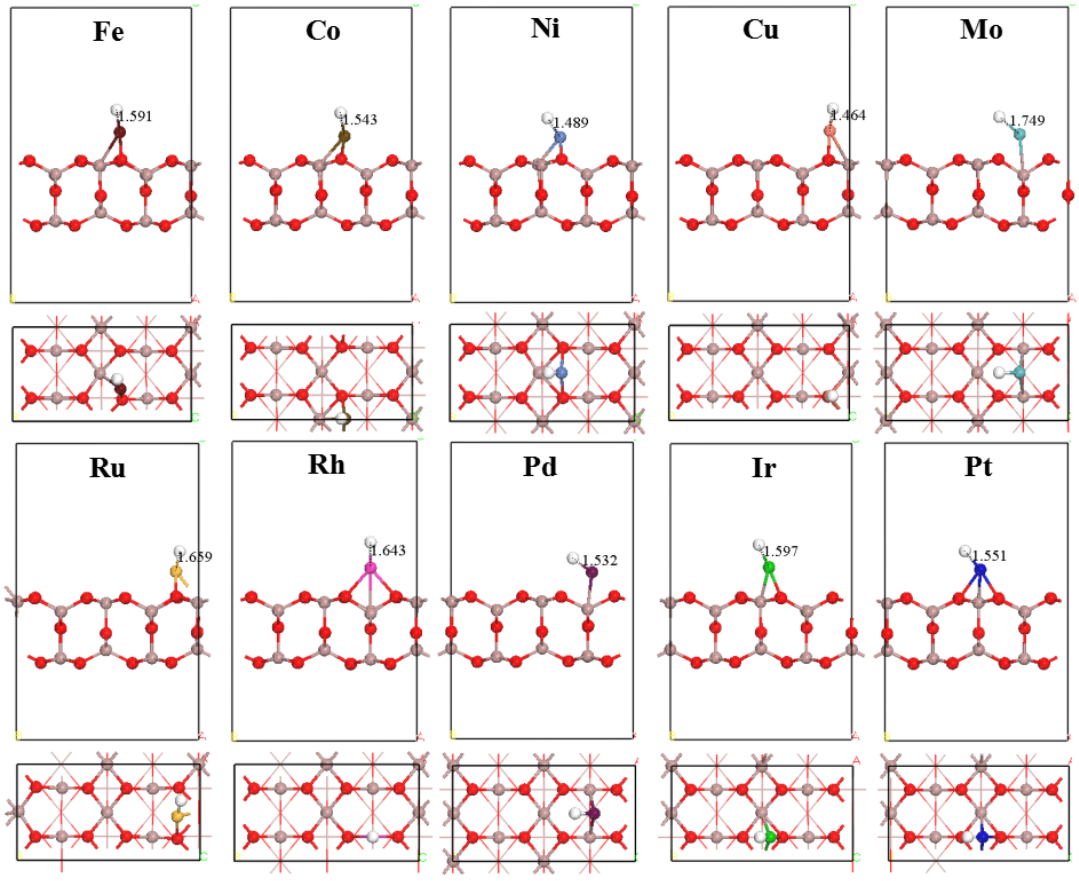

Fig. S4 Top-views and side-views of H adsorption structures of various TM atom adsorbed Ga_2O_3 monolayers.

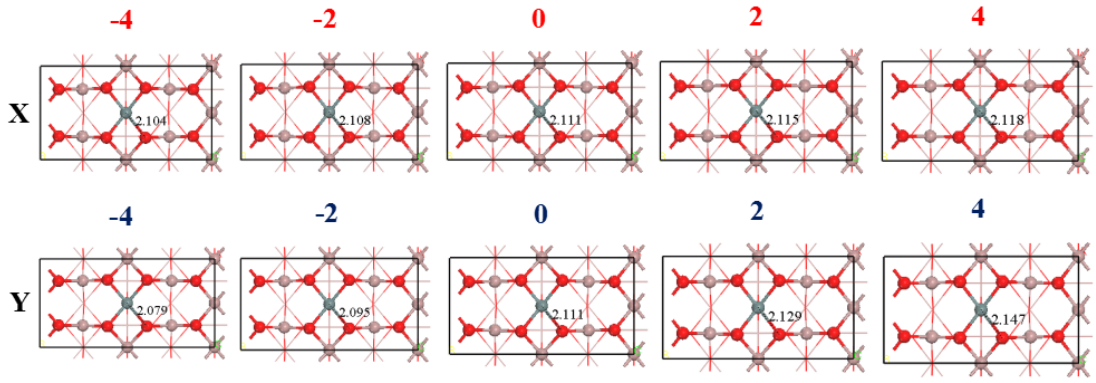

Fig. S5 Top-views of structures of Sn doped Ga_2O_3 monolayers with the strain from -4% to 4% in X direction and Y direction.

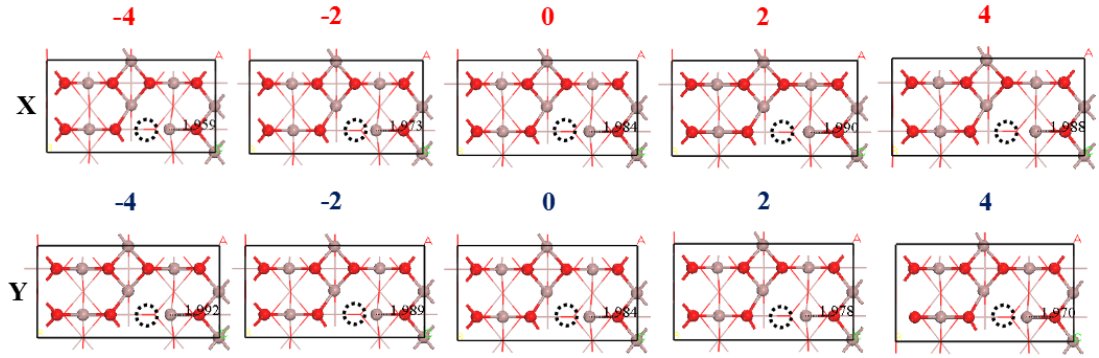

Fig. S6 Top-views of structures of O-V-Ga_2O_3 monolayers with the strain from -4% to 4% in X direction and Y direction.

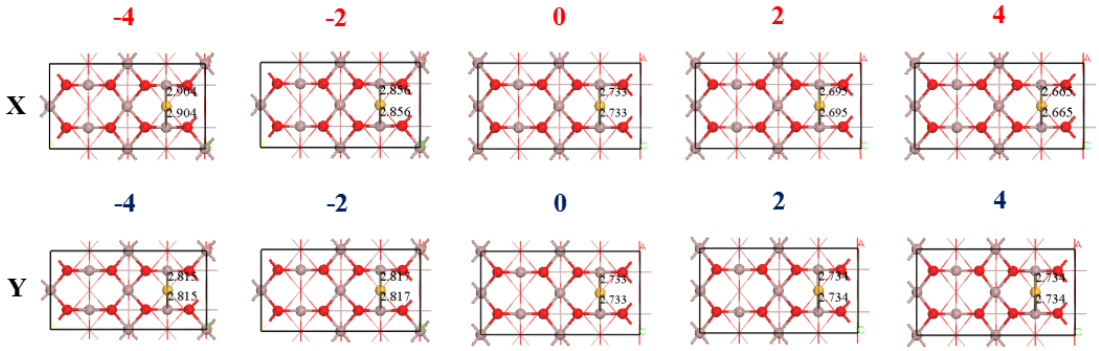

Fig. S7 Top-views of structures of Ru-Ga_2O_3 monolayers with the strain from -4% to 4% in X direction and Y direction.

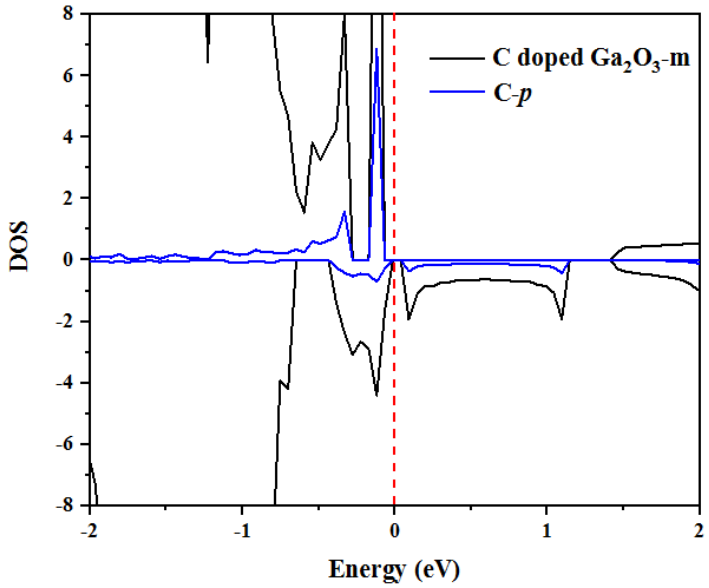

Fig. S8 The partial density of states (PDOS) of C doped Ga_2O_3-m.