Supplementary Information

Modulation in structural and electronic properties of 2D Ga_2O_3 by chemical passivation

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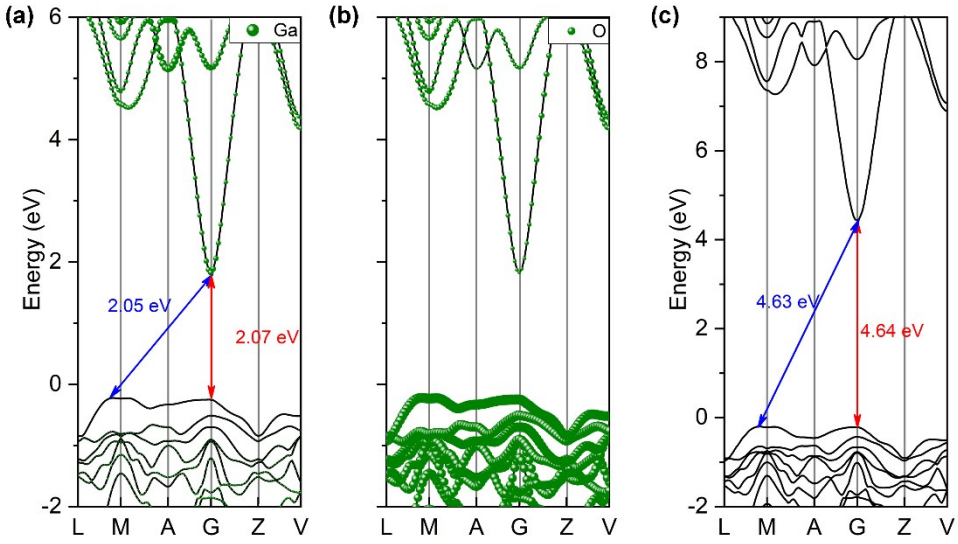

Fig. S1 Band structures of the bulk β-Ga_2O_3 calculated by PBE (a), (b) and HSE06 functional (c)

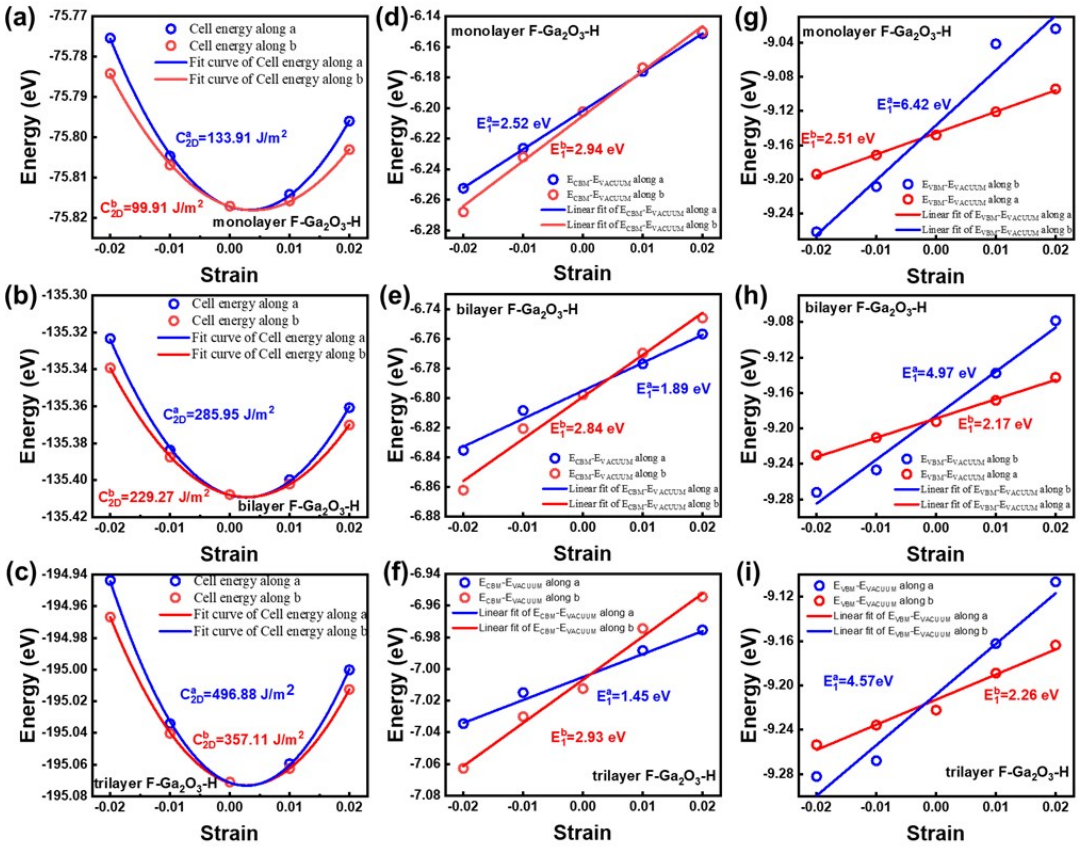

Fig. S2 Energy-strain relationship along a and b directions for monolayer (a), bilayer (b), and (c) trilayer 2D F-Ga_2O_3-H. Shifts of conduction band and valence band under uniaxial strain for 2D F-Ga_2O_3-H with different layers: (d) and (g) monolayer, (e) and (h) bilayer, (e) and (h) trilayer.

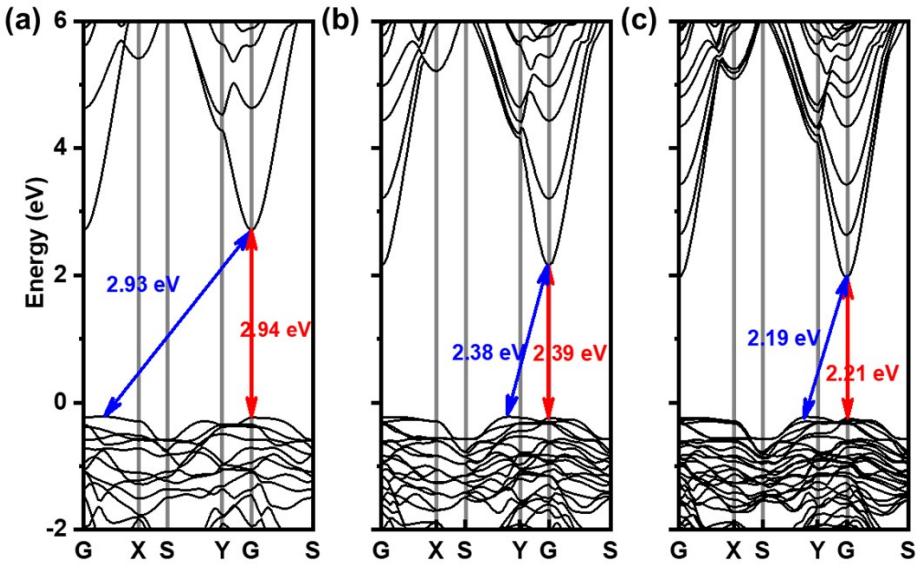

Fig. S3 Band structures of 2D F-Ga_2O_3-H with different layers: (a) monolayer, (b) bilayer, (c) trilayer