Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information for

Theoretical Insights into the Two-Dimensional Gallium Oxide Monolayer for Adsorption and Gas Sensing of C_4F_7N Decomposition Products

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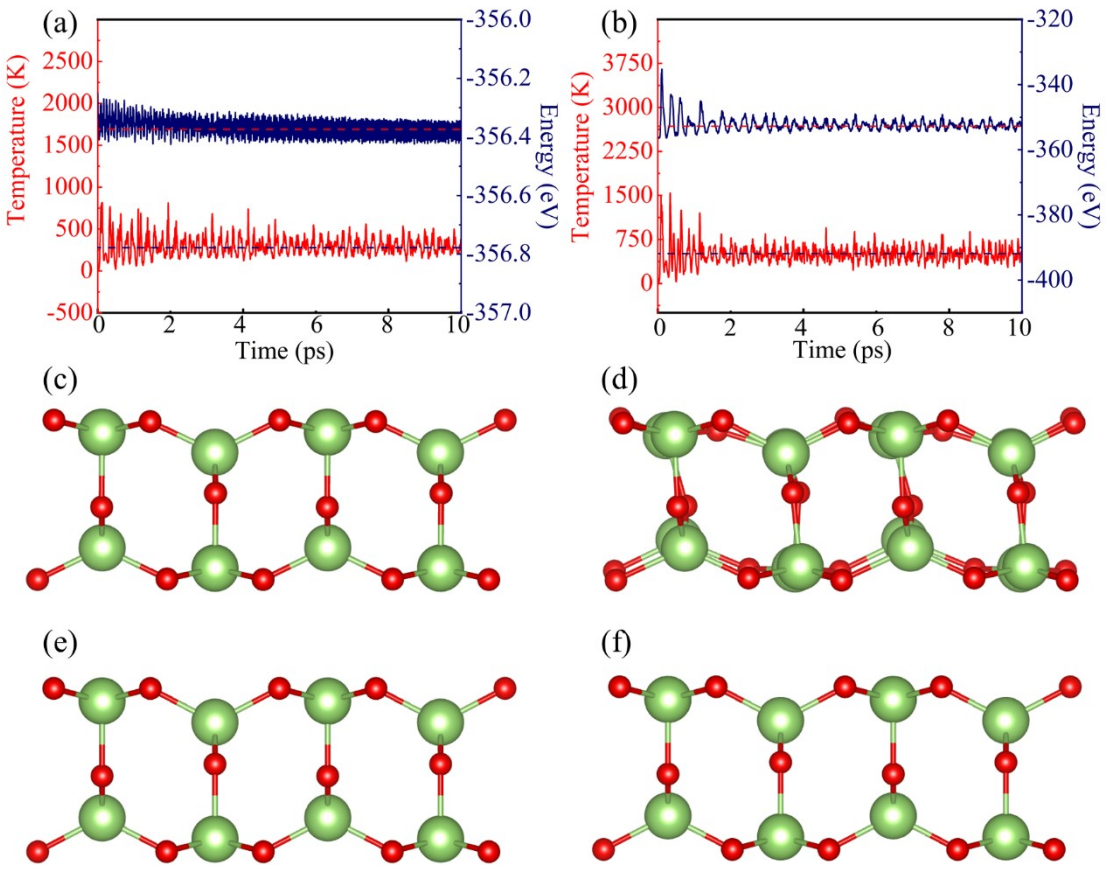

Fig. S1 Variations of temperature and energy *versus* the MD simulation time at (a) 300 K and (b) 500 K for pristine 2D Ga_2O_3. Atomic structures of 2D Ga_2O_3 after 10 ps AIMD simulation at (c) 300 K and (d) 500 K and (e-f) further geometry relaxation.

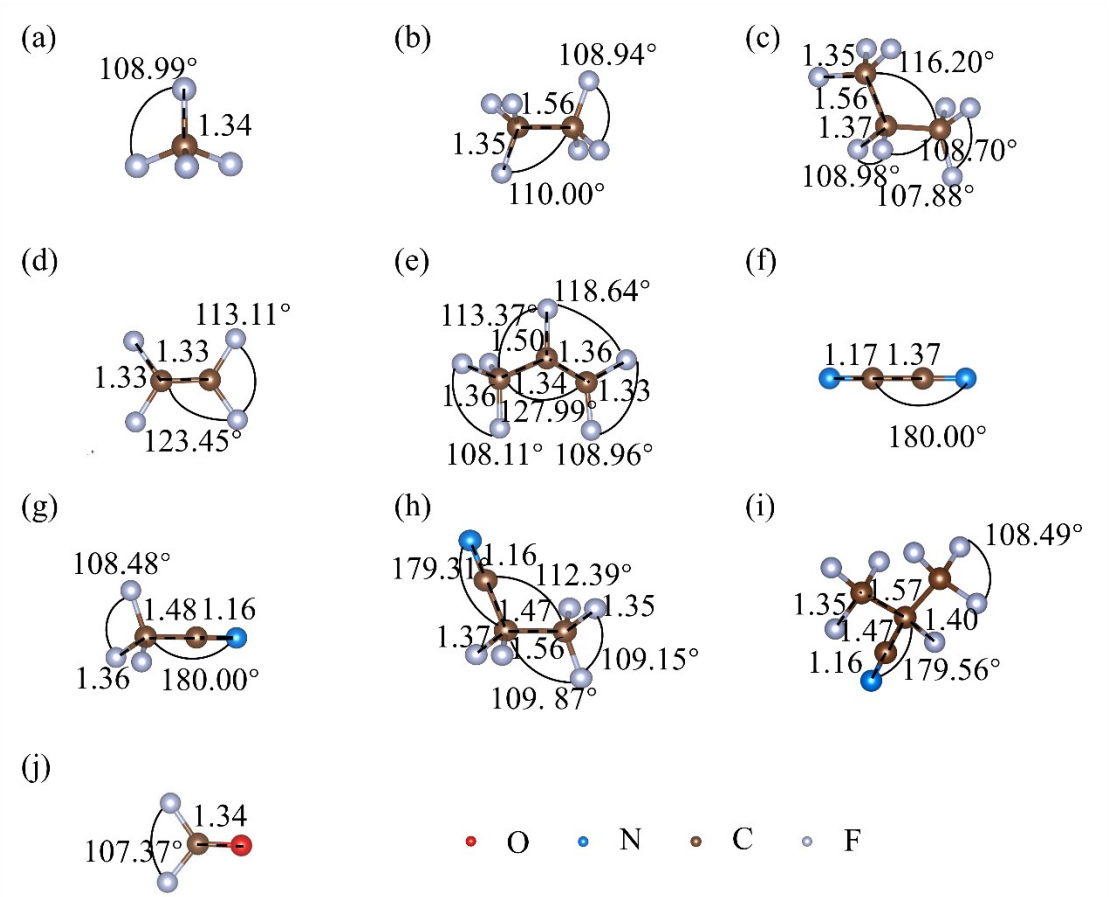

Fig. S2 Optimized atomic structures of (a) CF_4, (b) C_2F_6, (c) C_3F_8, (d) C_2F_4, (e) C_3F_6, (f) C_2N_2, (g) C_2F_3N, (h) C_3F_5N, (i) C_4F_7N, (j) COF_2.

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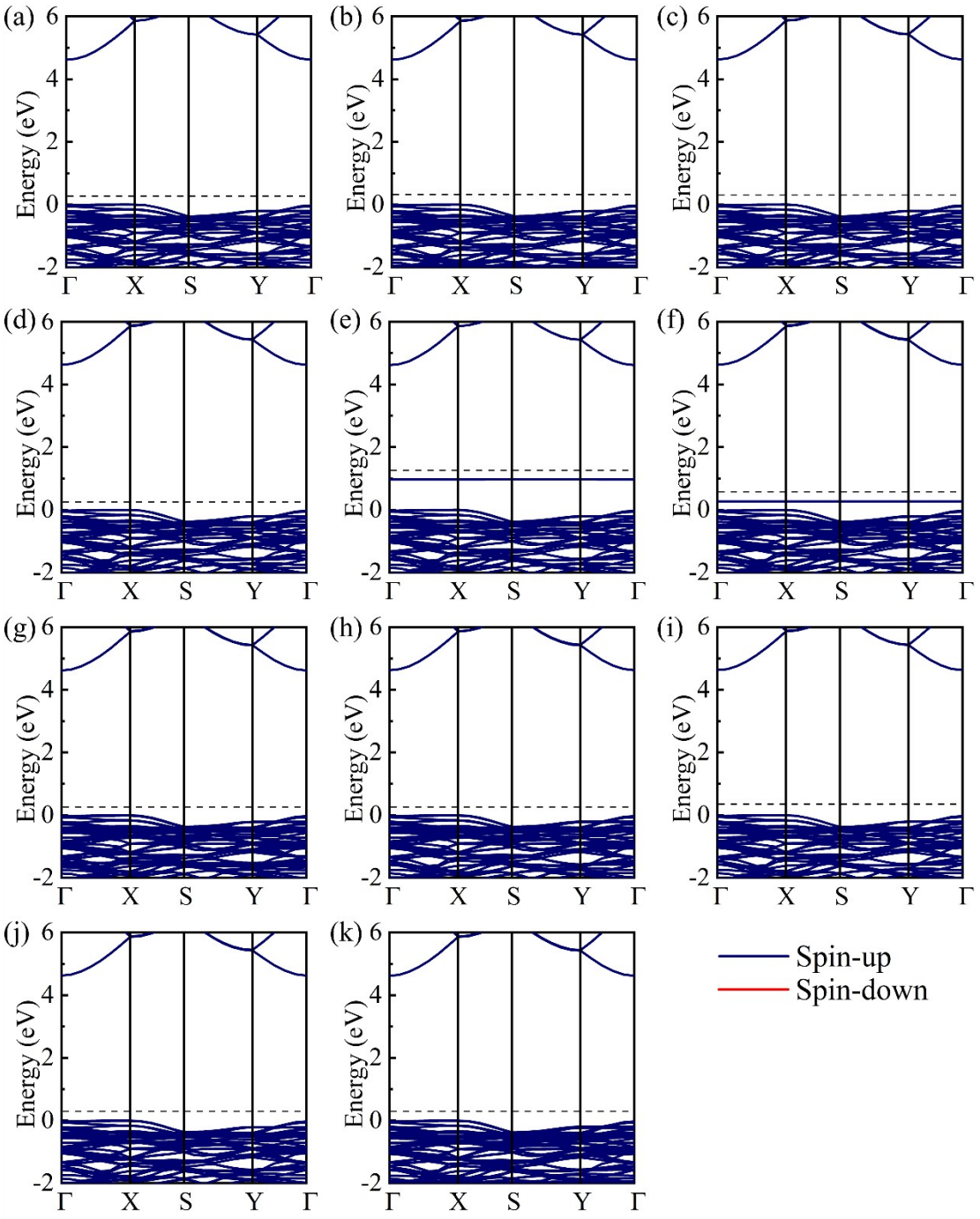

Fig. S3 Band structures of (a) pristine Ga_2O_3, and Ga_2O_3 adsorbed by (b) CF_4, (c) C_2F_6, (d) C_3F_8, (e) C_2F_4, (f) C_3F_6, (g) C_2N_2, (h) C_2F_3N, (i) C_3F_5N, (j) C_4F_7N, and (k) COF_2. The black dashed lines represent the E_F.

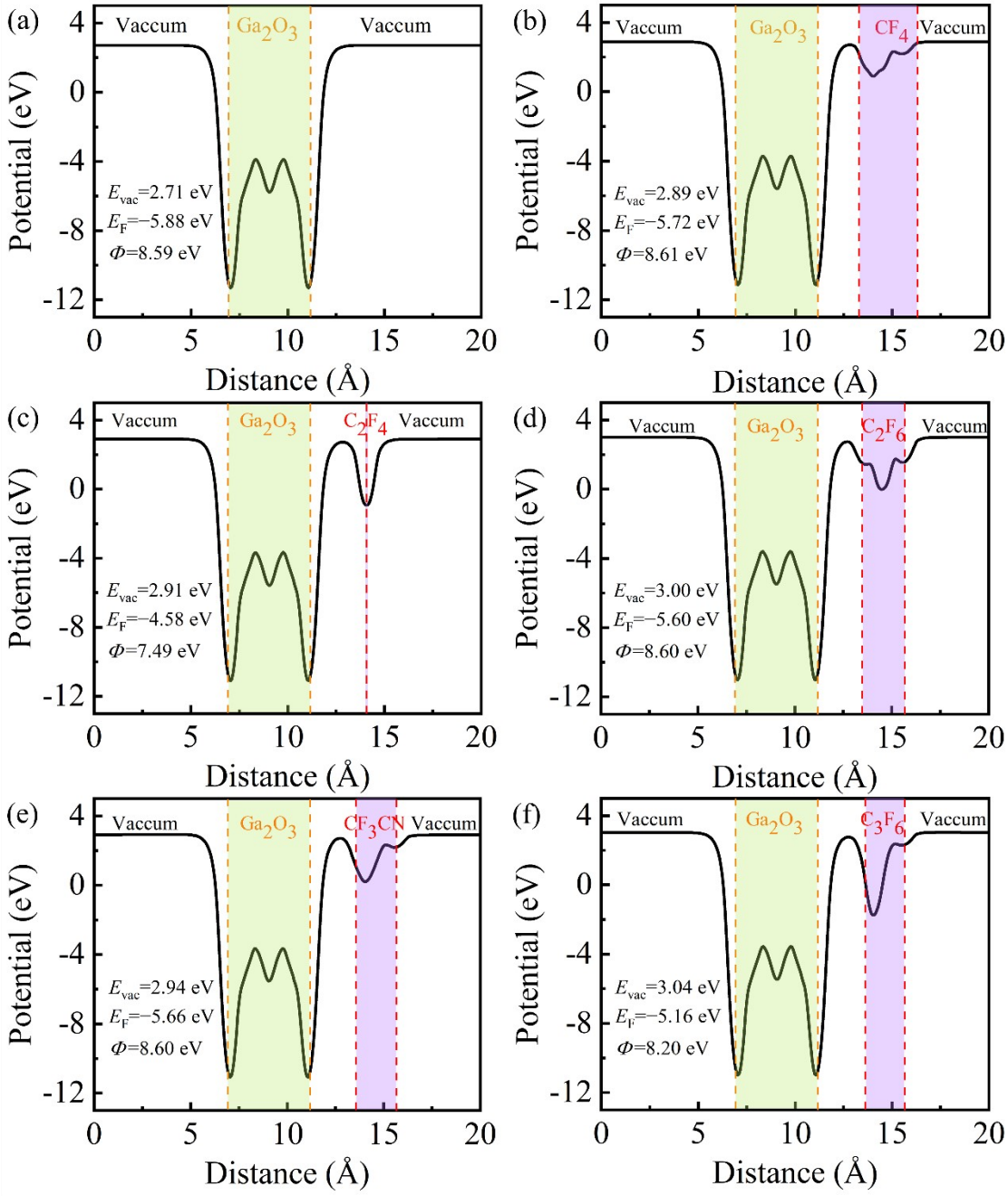

Fig. S4 Work function of (a) pristine Ga_2O_3, and Ga_2O_3 adsorbed by (b) CF_4, (c) C_2F_4, (d) C_2F_6, (e) C_2F_3N, (f) C_3F_6.

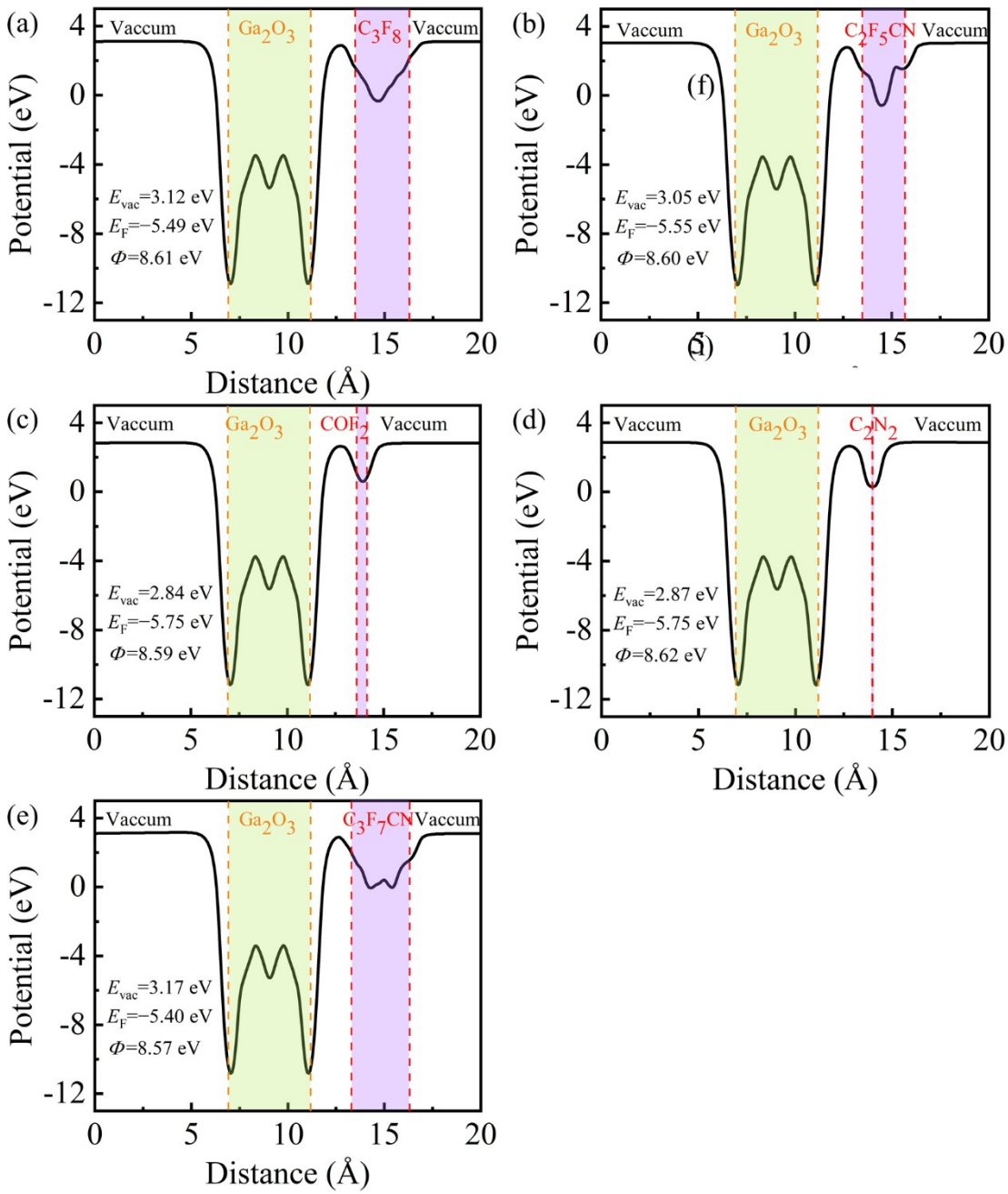

Fig. S5 Work function of Ga_2O_3 adsorbed by (a) C_3F_8, (b) C_3F_5N, (c) COF_2, (d) C_2N_2 and (e) C_4F_7N.

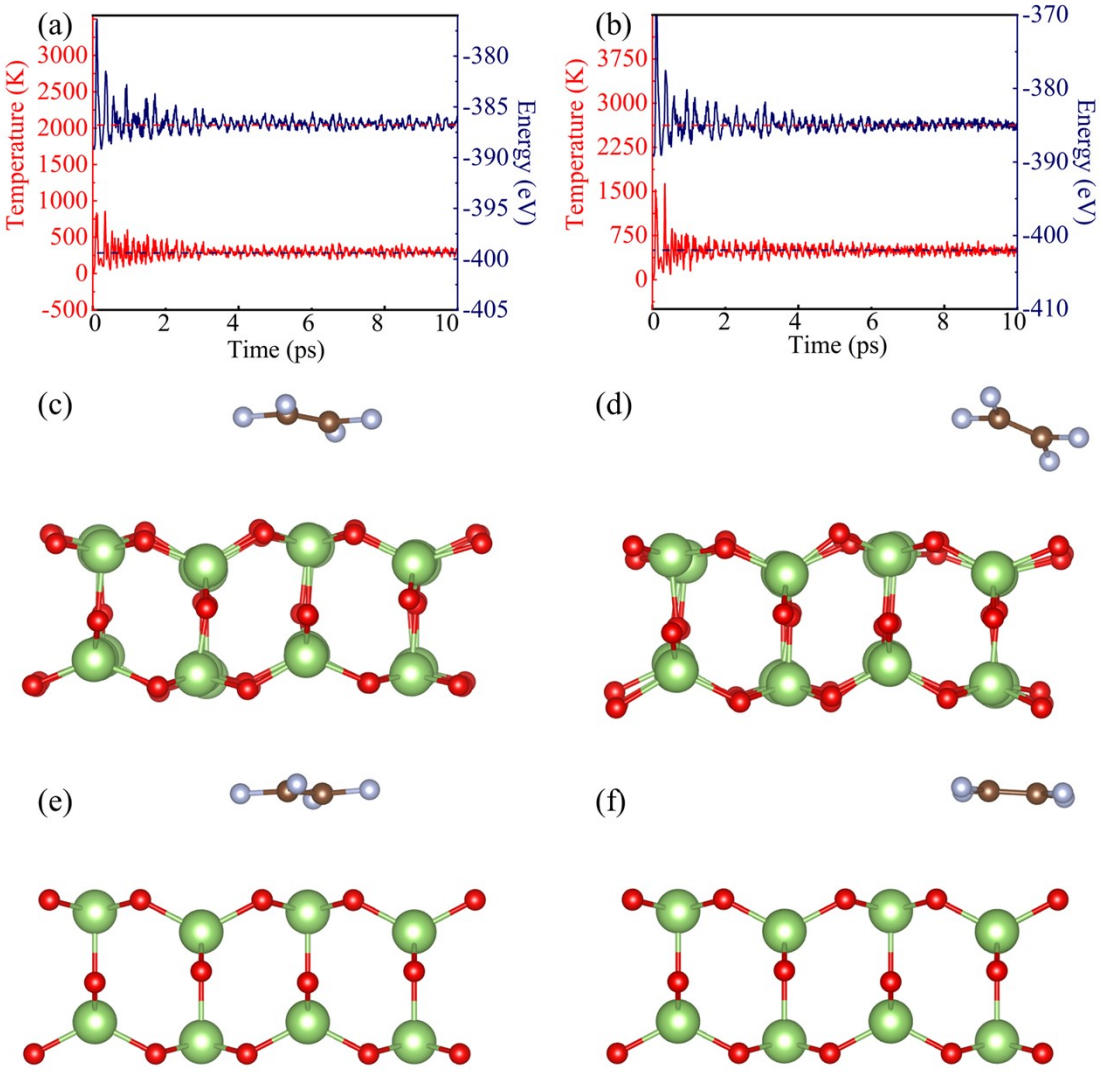

Fig. S6 Variations of temperature and energy *versus* the AIMD simulation time at (a) 300 K and (b) 500 K for C_2F_4@Ga_2O_3. Atomic structures of C_2F_4@Ga_2O_3 after 10 ps AIMD simulation at (c) 300 K and (d) 500 K and (e-f) further geometry relaxation.

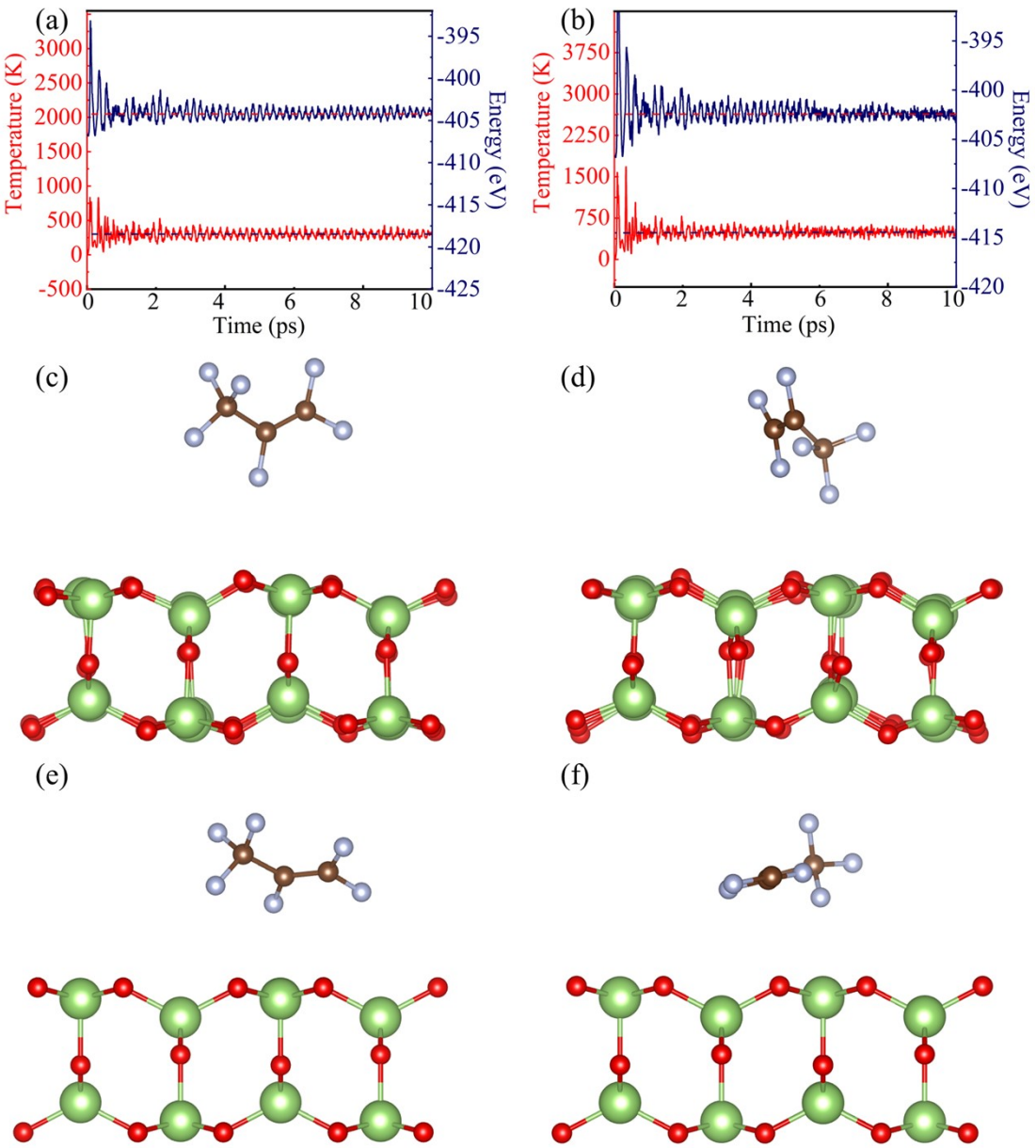

Fig. S7 Variations of temperature and energy *versus* the AIMD simulation time at (a) 300 K and (b) 500 K for C_3F_6@Ga_2O_3. Atomic structures of C_3F_6@Ga_2O_3 after 10 ps AIMD simulation at (c) 300 K and (d) 500 K and (e-f) further geometry relaxation.

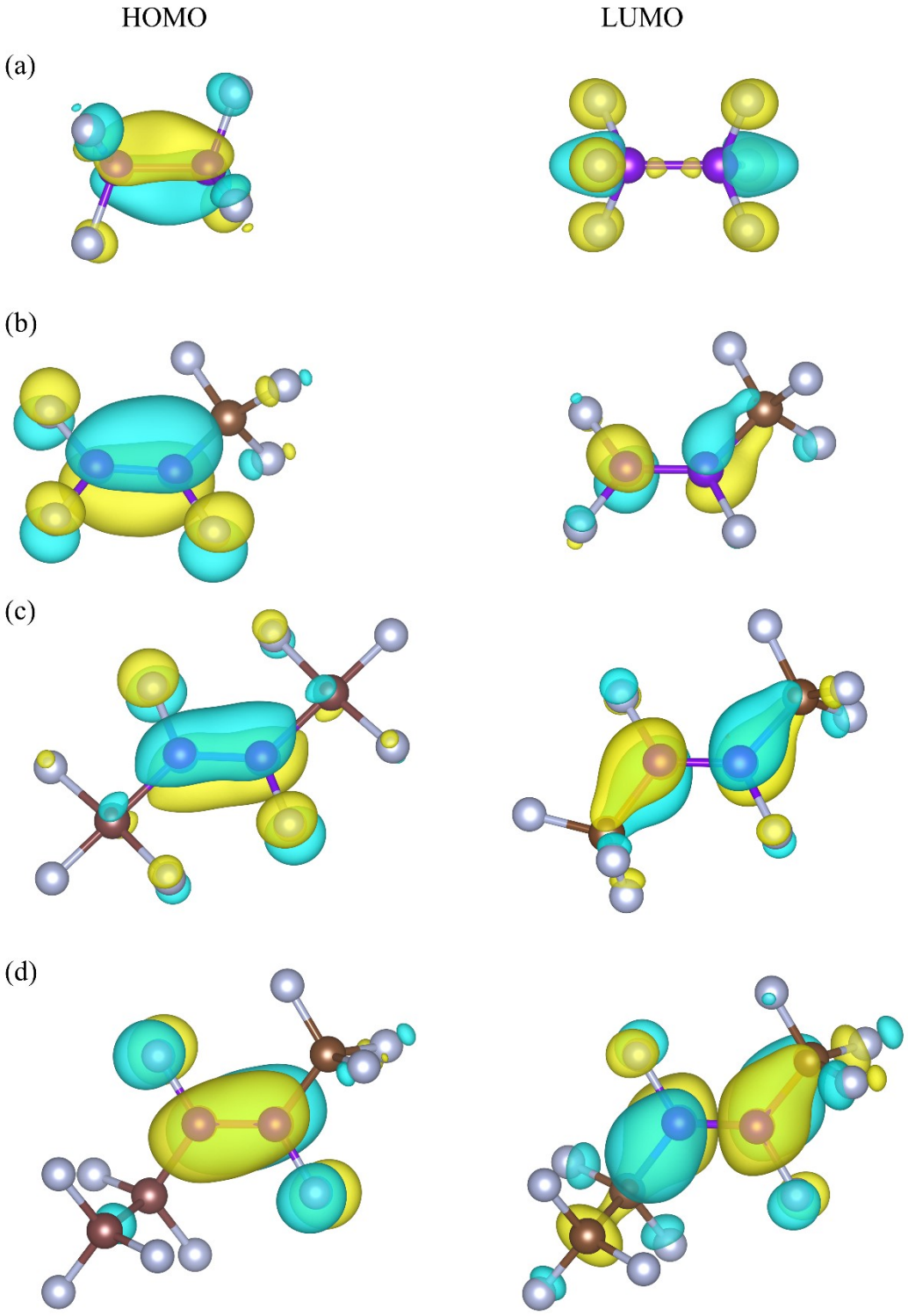

Fig. S8 The highest occupied orbital (HOMO) and lowest unoccupied orbital (LUMO) of (a) C_2F_4, (b) C_3F_6, (c) C_4F_8, (d) C_5F_{10}.

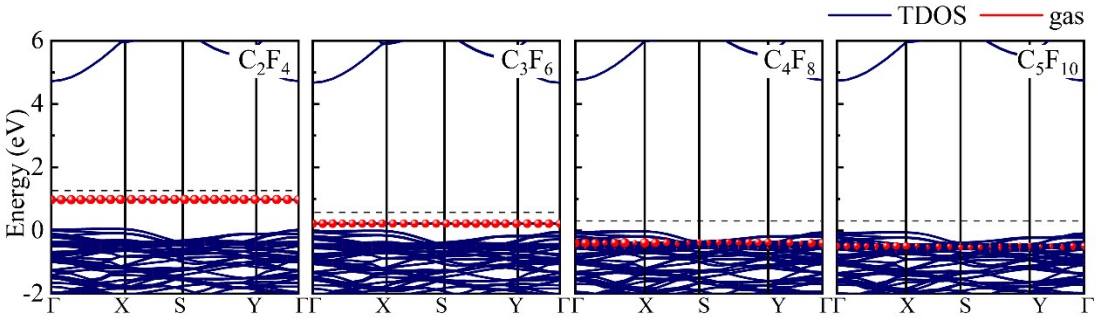

Fig. S9 Orbital-resolved band structures of C_xF_{2x}@Ga_2O_3. The black dashed lines represent the E_F.

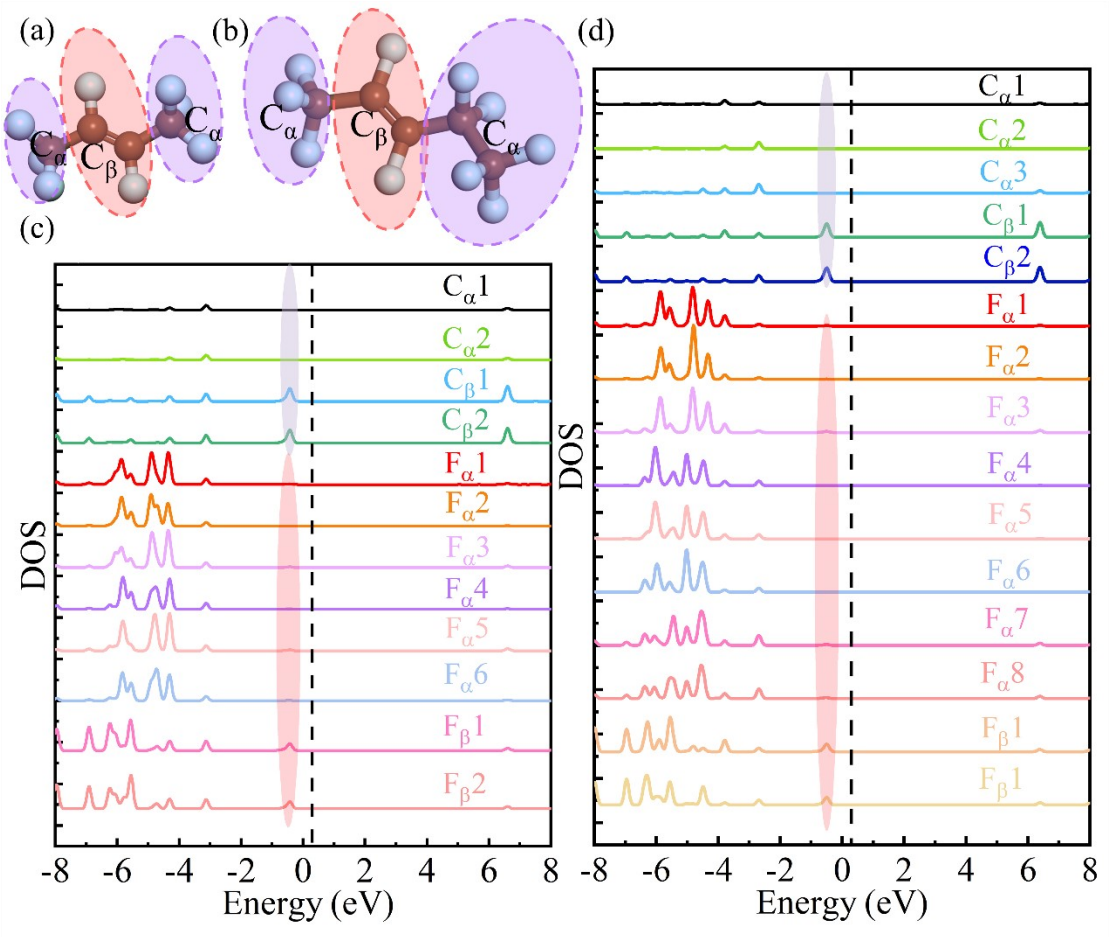

Fig. S10 Atomic structures of (a) C_4F_8 and (b) C_5F_{10}. PDOS of (c) C_4F_8@Ga_2O_3 and (d) C_5F_{10}@Ga_2O_3 contributed by C and N atoms. The black dashed lines represent the E_F.

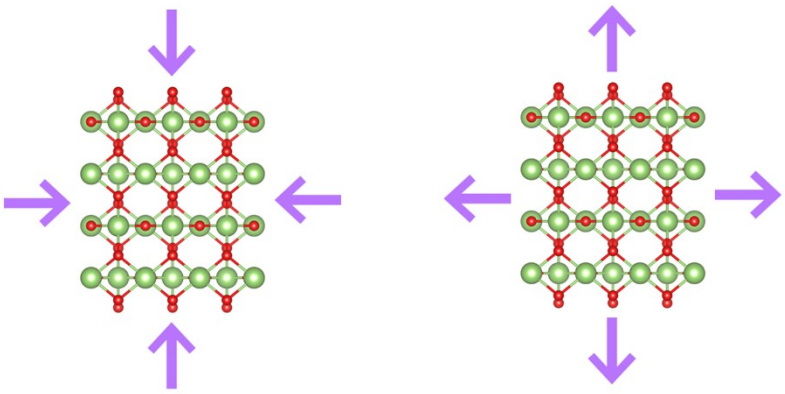

Fig. S11 Schematic illustration of applying compressive and tensile biaxial strain to pristine Ga_2O_3 and gas@Ga_2O_3.

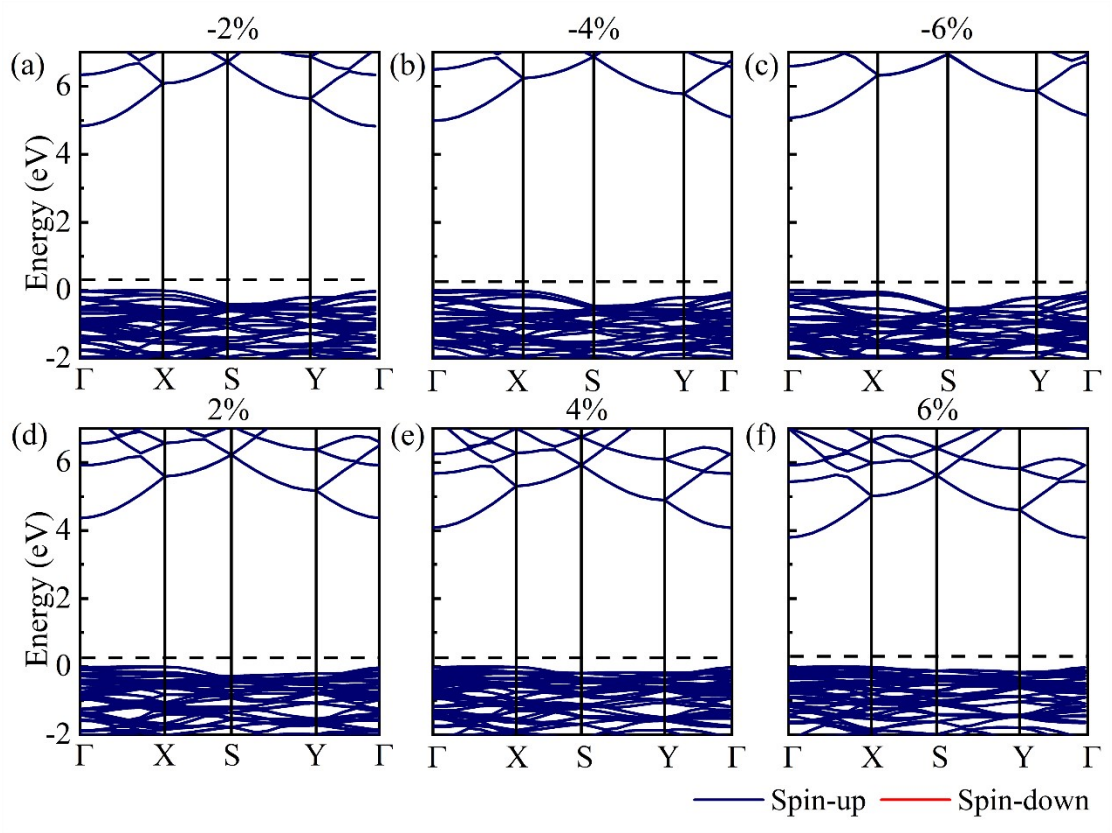

Fig. S12 Band structures of pristine Ga_2O_3 under biaxial strain. The black dashed lines represent the E_F.

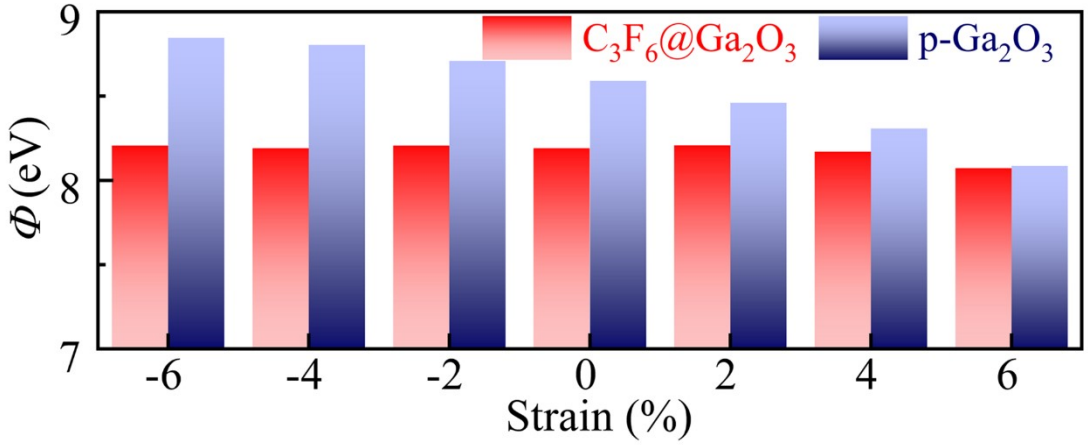

Fig. S13 Strain-induced work function of pristine Ga_2O_3 and $C_3F_6@Ga_2O_3$.

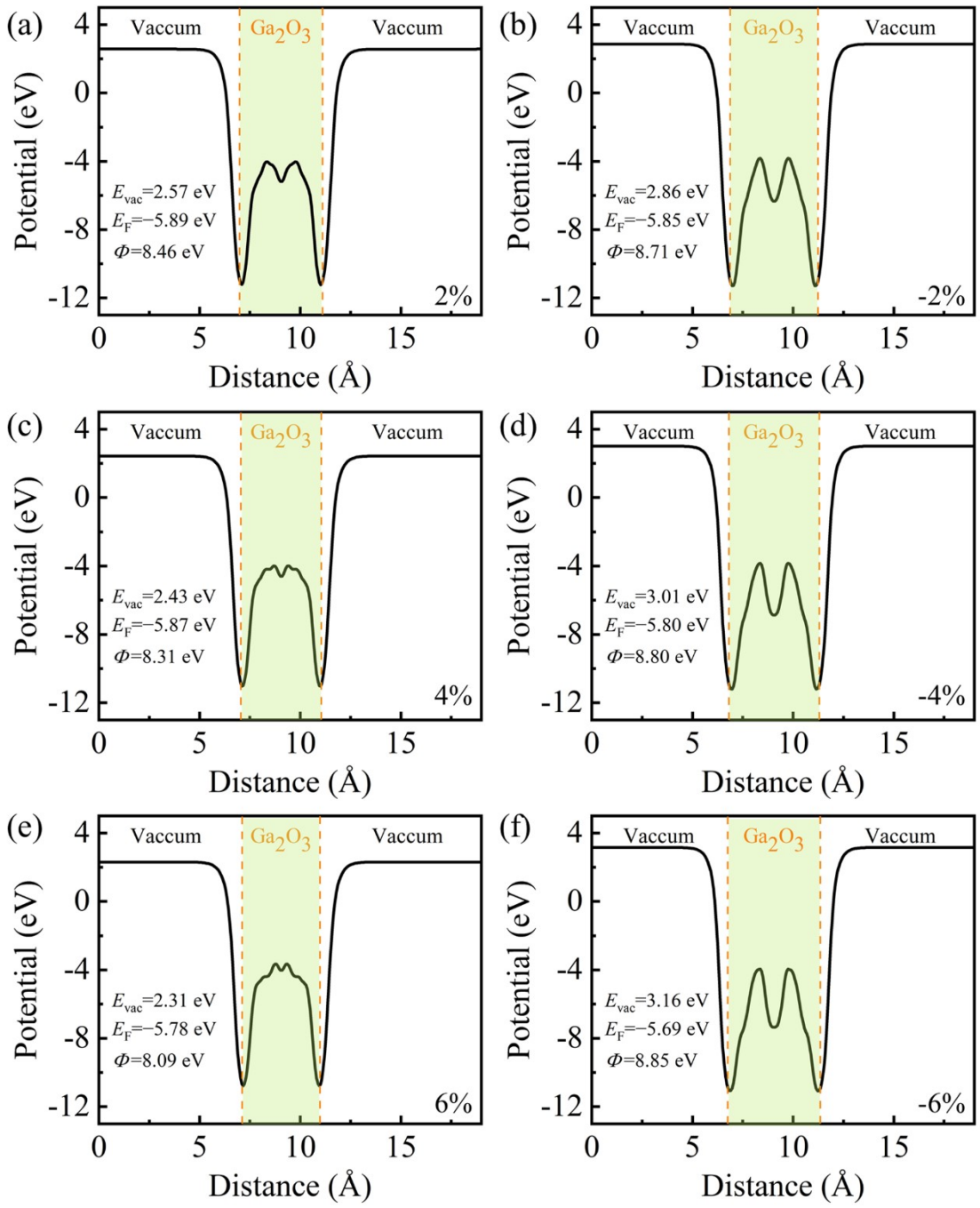

Fig. S14 Work function of pristine Ga_2O_3 under biaxial strain.

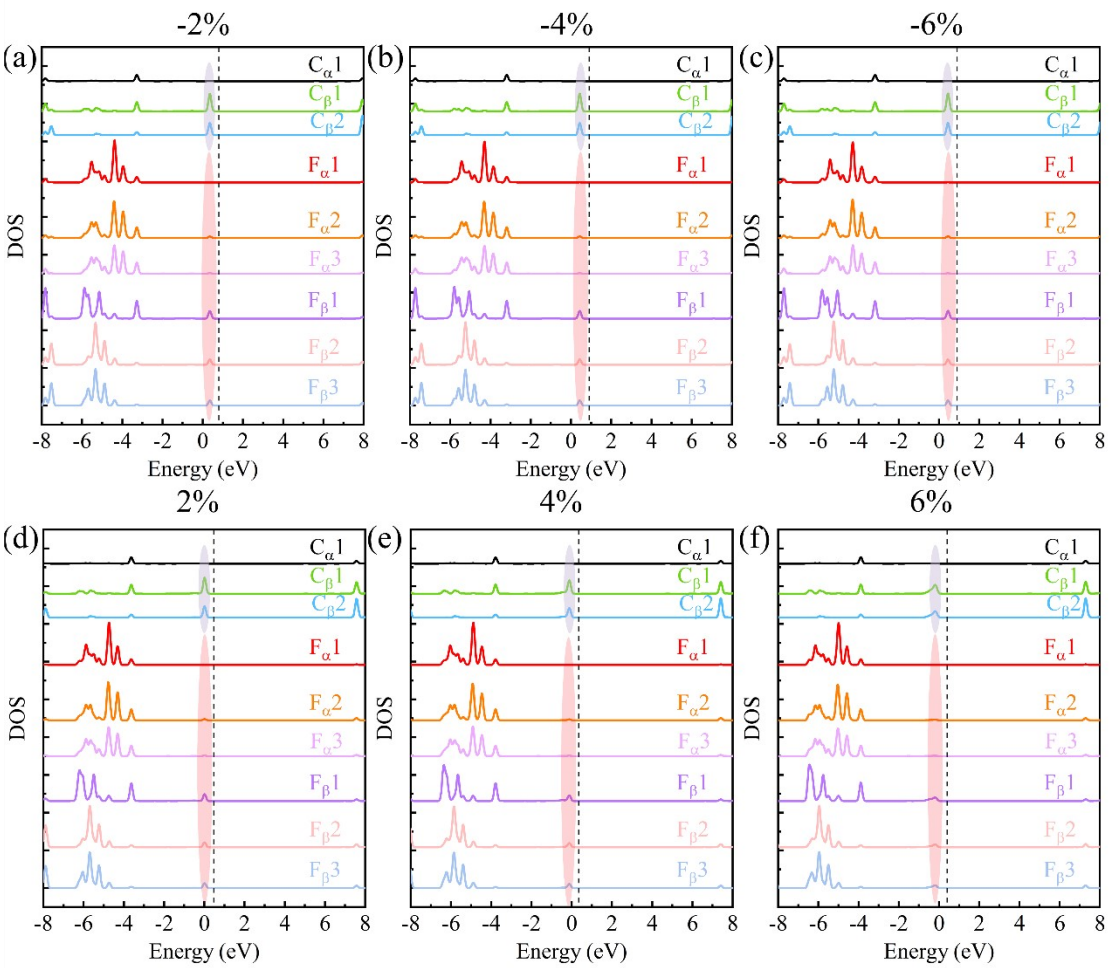

Fig. S15 PDOS of pristine C_3F_6@Ga_2O_3 under biaxial strain. The black dashed lines represent the E_F.

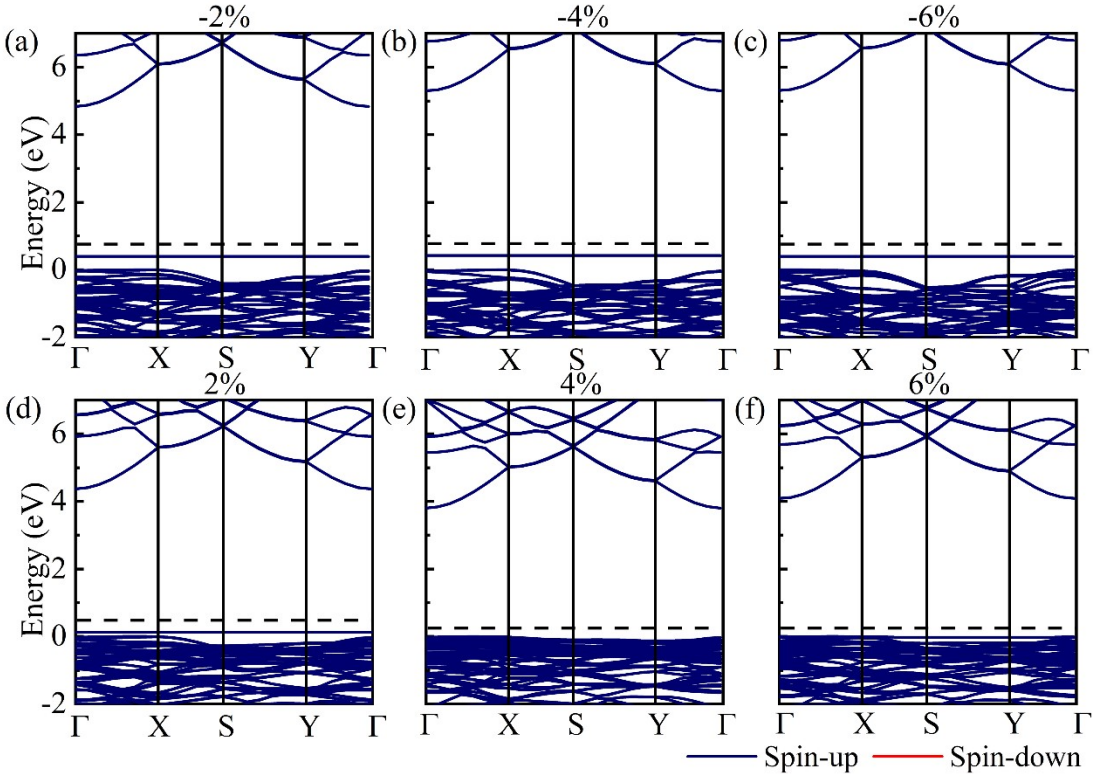

Fig. S16 Band structures of C_3F_6@Ga_2O_3 under biaxial strain. The black dashed lines represent the E_F.

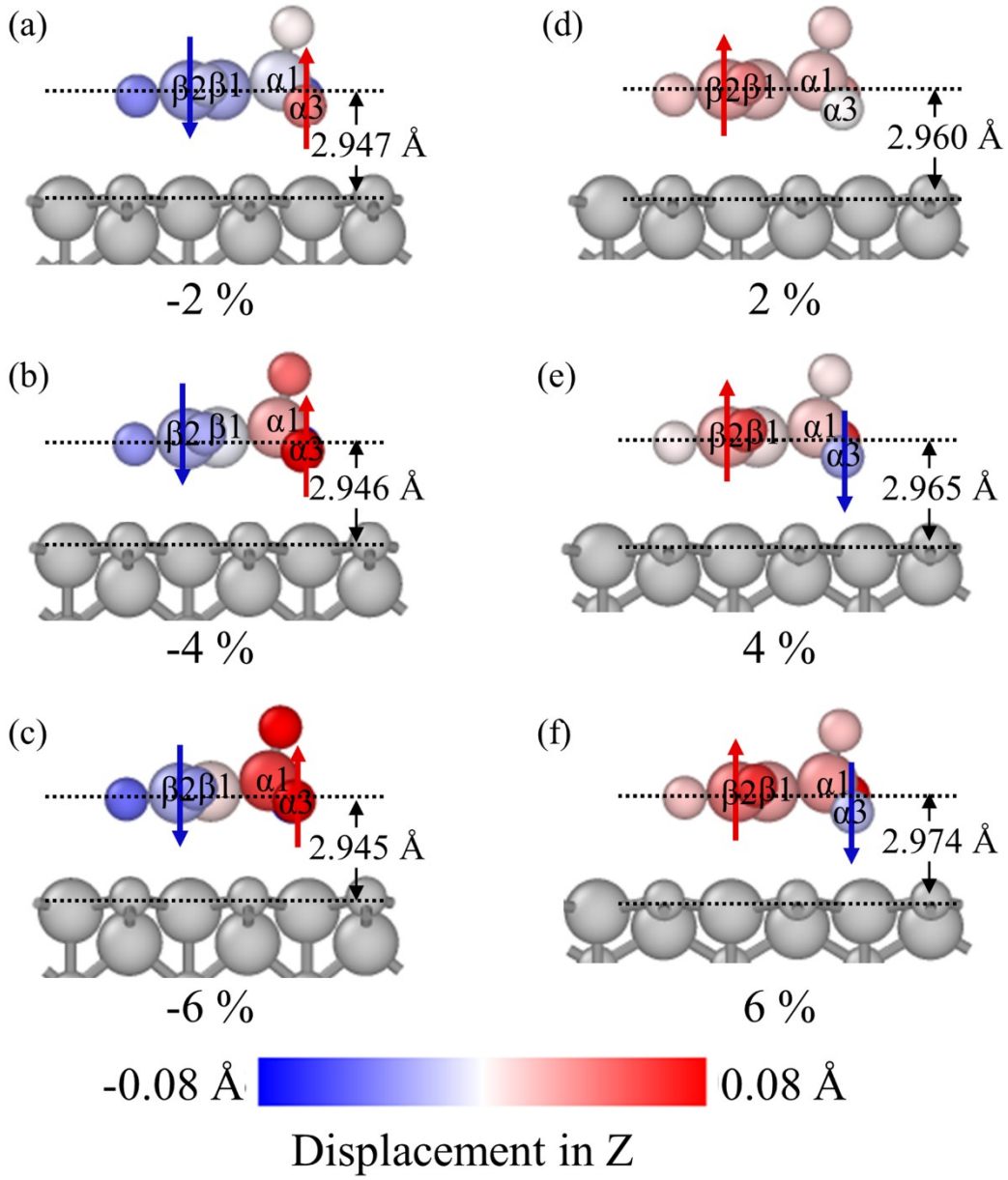

Fig. S17 Local atomic configuration of the C_3F_6@Ga_2O_3 with lattice strain from -6% to +6%. The atoms are color-coded by the displacement in *z* direction with the reference of the unstrained C_3F_6@Ga_2O_3 systems. The -6% and +6% cases are the same in Fig. 6 in the main paper.

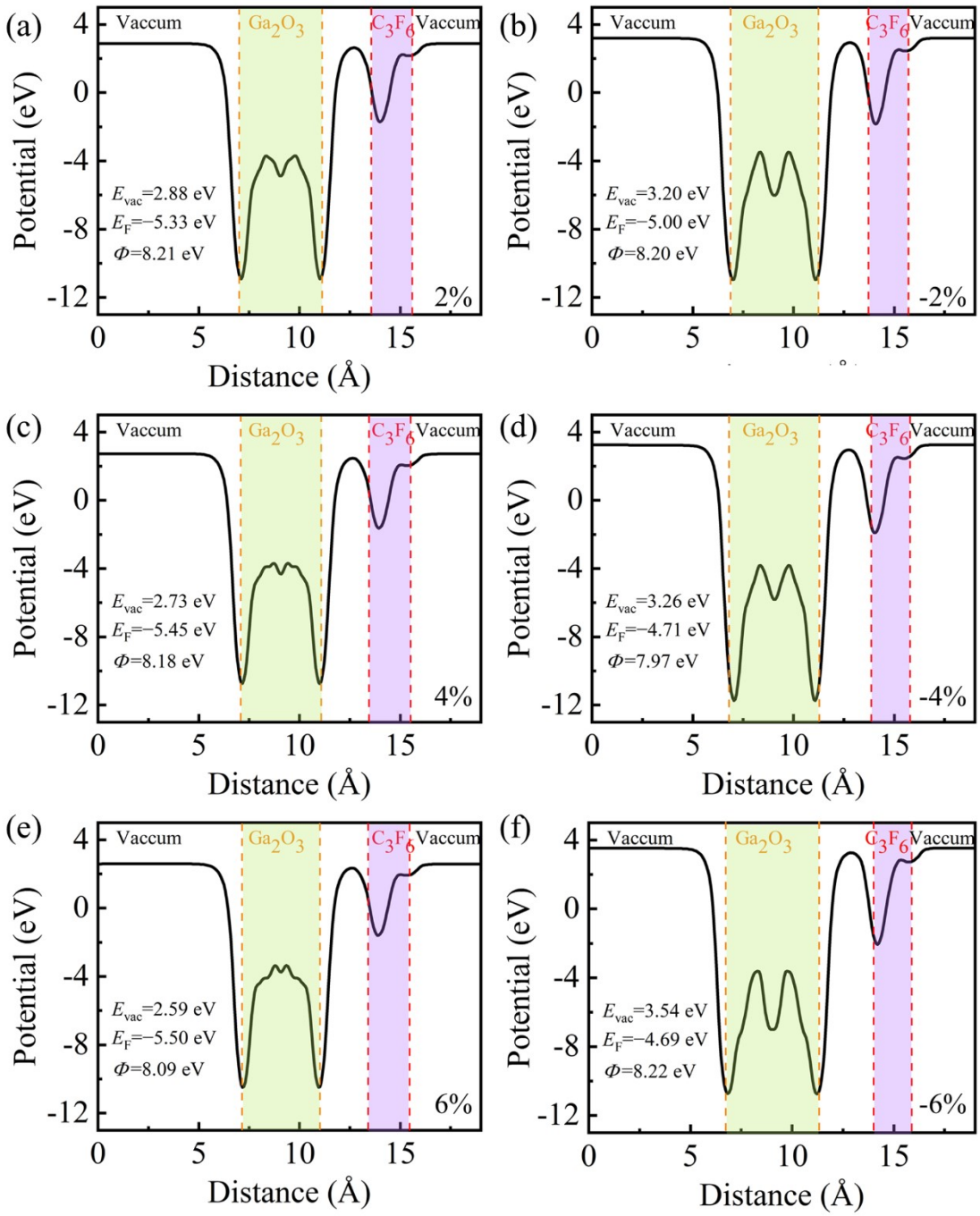

Fig. S18 Work function of C_3F_6@Ga_2O_3 under biaxial strain.

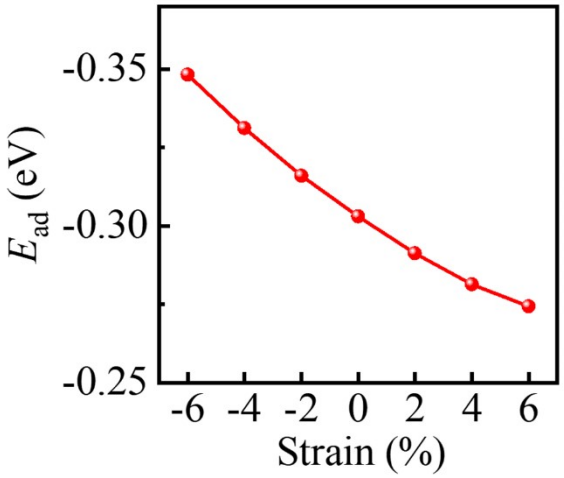

Fig. S19 Adsorption energy *versus* the applied biaxial strain for C_2F_4@Ga_2O_3.

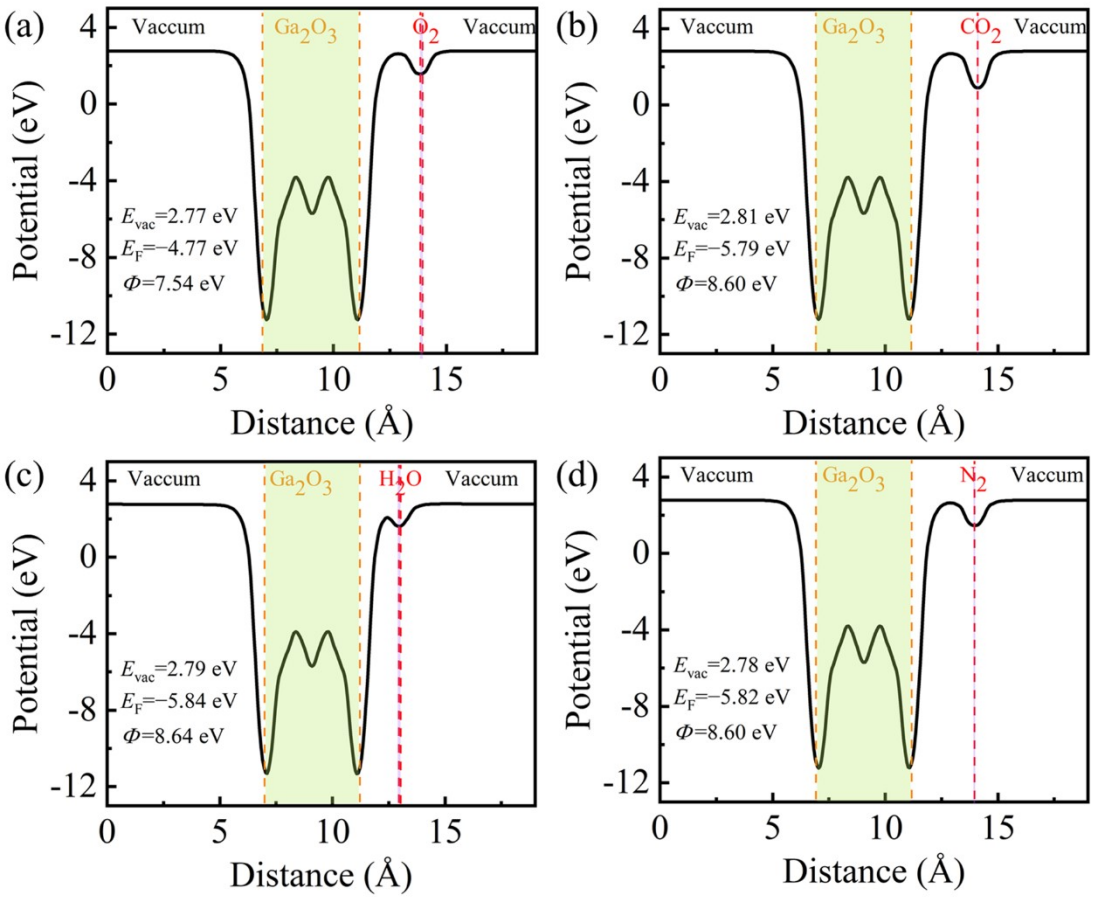

Fig. S20 Work function of (a) O_2, (b) CO_2, (c) H_2O and (d) N_2 adsorbed Ga_2O_3.

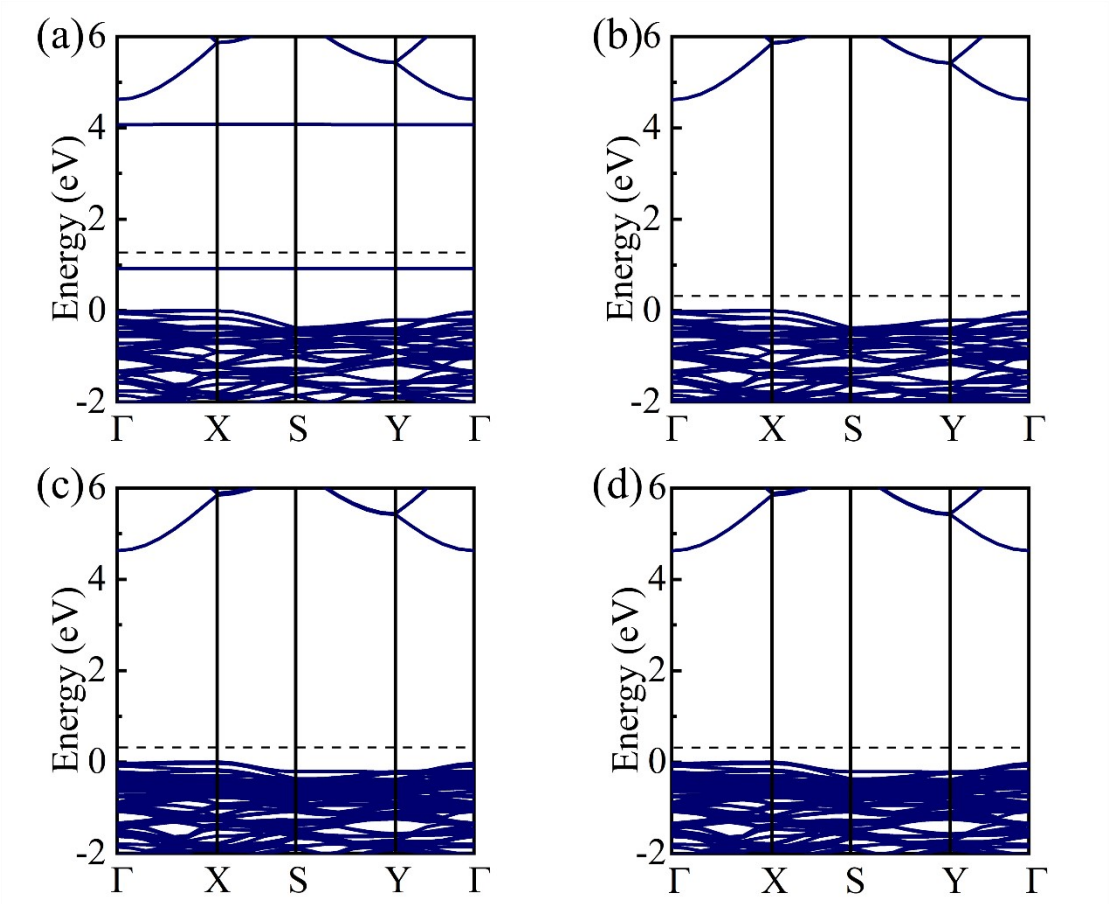

Fig. S21 Band structures of (a) O_2, (b) CO_2, (c) H_2O and (d) N_2 adsorbed Ga_2O_3. The black dashed lines represent the E_F.

Table S1 Calculated adsorption energy (E_{ad}), adsorption height (H), charge transfer (ΔQ), recovery time (τ), and work function (Φ) of all adsorption systems.

System	E_{ad} (eV)	H (Å)	ΔQ (e)	τ (s)	Φ (eV)
O_2	-1.25	2.66	0.0157	9.83×10^{8}	7.54
CO_2	-0.15	2.95	-0.0008	3.30×10^{-10}	8.60
H_2O	-0.32	1.82	0.0112	2.37×10^{-7}	8.64
N_2	-0.16	2.79	0.0096	4.86×10^{-10}	8.60