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Supplementary information:

Facet-Engineered CeO₂/Graphene Composites for Enhanced NO₂ Gas-Sensing

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Figure S1. The SEM and TEM images of CeO₂/Graphene composites prepared with EG/H₂O volume ratios of 0:40. (a, b: SEM images, c, d: TEM images)



Figure S2. Elemental maps of the CeO₂/graphene nanocomposite.



Figure S3. Calculated surface energy of the CeO₂ {111} and {100} planes as well as adsorption energy of ethylene glycol: (a, b) Clean surface; (c, d) Ethylene glycol-covered surface (E_{surf} =surface energy and E_{ads} =absorption energy).



Figure S4. The response curves to 50 ppm NO₂ of CeO₂/Graphene composites prepared with EG/H₂O volume ratios of 0:40 at operating temperature of 25°C, 50°C, 80°C and 100°C.



Figure S5. Response and recovery curves of $CeO_2\{111\}$ /graphene composites prepared with different EG/H₂O volume ratios: (a) 0:40, (b) 10:30, (d) 30:10, and (e) 40:0. The concentration of NO₂ adopted is in the range of 10-200 ppm, and the measurements are done at room temperature.



Figure S6. The sensitivity of the CeO₂/Graphene composites to 200 ppm NO₂ measured every days. (b: EG/H₂O=10:30, c: EG/H₂O=20:20, d:EG/H₂O=30:10, and e: EG/H₂O=40:0)



Figure S7. The response of CeO₂/Graphene sensor to 100 ppm several possible interferential gases. (Magenta: The previous work^[20], Green: Our work)



Figure S8. Sensitivity of the pure CeO_2 nanoparticles prepared with different volume ratios of the EG/H₂O for 10-200 ppm NO₂ at room temperature.(a: 0:40, b: 10:30, c: 20:20, d: 30:10, and e: 40:0).



Figure S9. Work function of the (a) $CeO_2\{111\}$ plane; (b) graphene; (c) $CeO_2\{100\}$ plane terminated with Ce; (d) $CeO_2\{100\}$ plane terminated with O.



Figure S10. Energy band configurations of $CeO_2\{111\}/graphene$ composites.(E_C : Conduction band, E_V : Valence band, and E_F : Fermi level)



Figure S11. The DOS and PDOS of (a, b) the CeO_2 {111} plane, (c, d) the {100}-Ce plane, respectively. The dashed lines indicate the Fermi level.