

Supporting Information for

Theoretical Study on Selective Adsorption, Synergistic Effects, and Conversion of NO₂ and SO₂ on Cu_g/PCN

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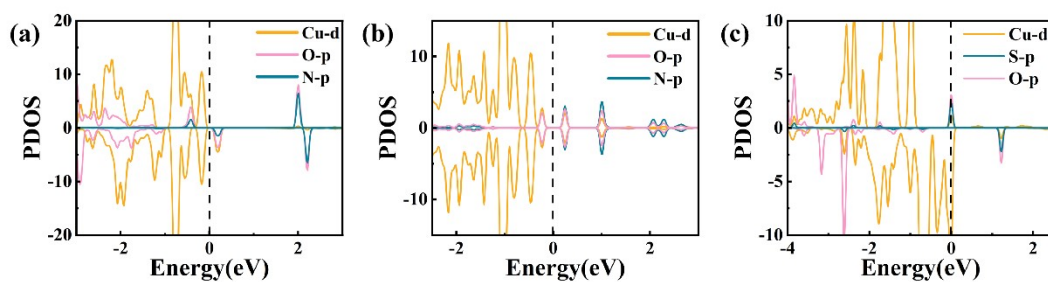


Fig. S1. Projected density of states (PDOS) for the adsorption of (a) 2NO₂, (b) 2NO, and (c) SO₂ on Cu_g/PCN. The Fermi level is set to 0 eV (black dashed line).

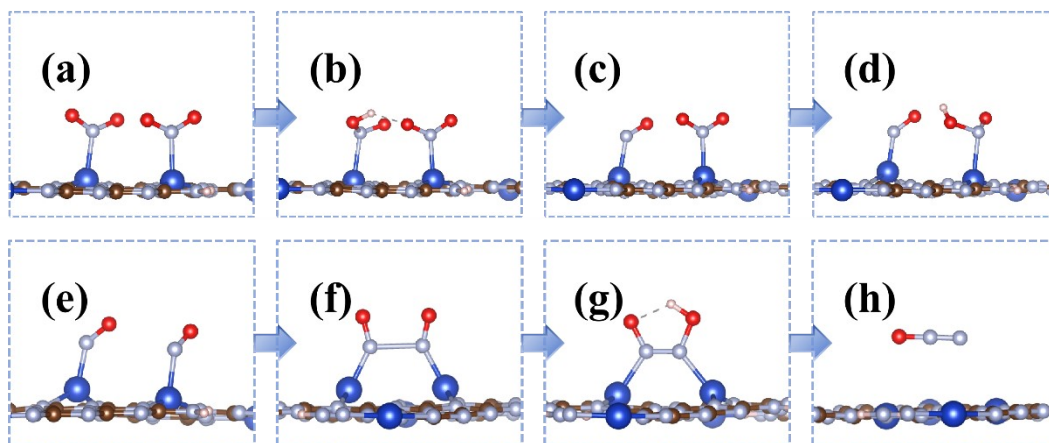


Fig. S2. Optimized structures of species involved in the NO_2 -to- N_2O reduction pathway on Cu_9/PCN . (a) $^*\text{NO}_2 + ^*\text{NO}_2$; (b) $^*\text{HNO}_2 + ^*\text{NO}_2$; (c) $^*\text{NO} + ^*\text{NO}_2$; (d) $^*\text{NO} + ^*\text{NO}_2\text{H}$; (e) $^*\text{NO} + ^*\text{NO}$; (f) $^*\text{NONO}$ (spontaneous N-N coupling from e; this configuration is identical to the directly adsorbed NO dimer shown in Fig. 1c); (g) $^*\text{NONOH}$; (h) $\text{N}_2\text{O}(\text{g})$ (after desorption). The arrow from (e) to (f) indicates the thermodynamically favored structural relaxation from two isolated $^*\text{NO}$ to the more stable bridging $^*\text{NONO}$ configuration.

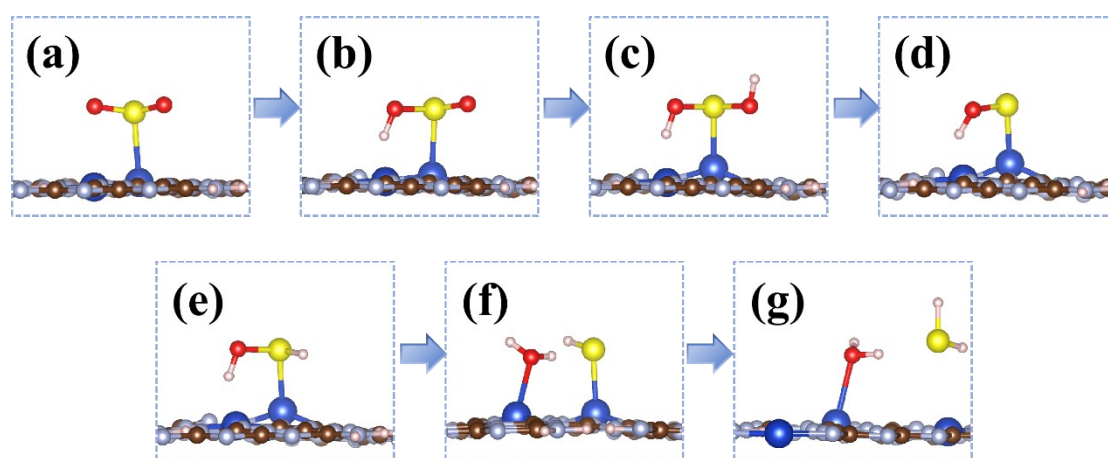


Fig. S3. Optimized structures of species involved in the SO_2 -to- H_2S reduction pathway on Cu_9/PCN . (a) $^*\text{SO}_2$; (b) $^*\text{HOSO}$; (c) $^*\text{S}(\text{OH})_2$; (d) $^*\text{SOH}$; (e) $^*\text{HSOH}$; (f) $^*\text{SH} + ^*\text{H}_2\text{O}$; (g) $\text{H}_2\text{S}(\text{g})$ (after desorption).

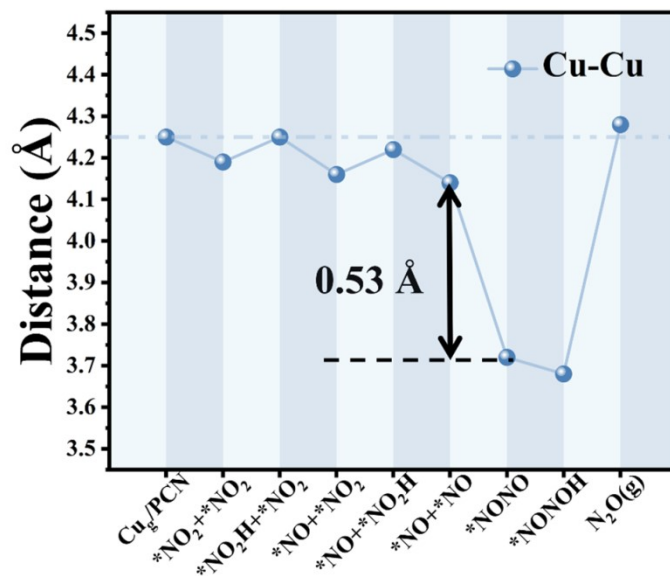


Fig. S4. Evolution of the Cu–Cu distance along the NO₂-to-N₂O reduction pathway on Cu₉/PCN. The distances correspond to the species shown in Figure S2. The dashed line indicates the Cu–Cu distance in pristine Cu₉/PCN (4.25 Å). The arrow highlights the contraction from two isolated *NO to the bridging *NONO configuration.

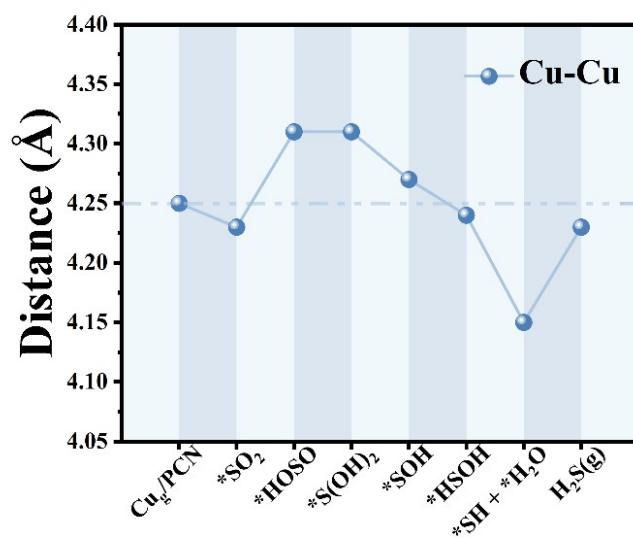


Fig. S5. Evolution of the Cu–Cu distance along the SO₂-to-H₂S reduction pathway on Cu₉/PCN. The distances correspond to the species shown in Figure S3. The dashed line indicates the Cu–Cu distance in pristine Cu₉/PCN (4.25 Å).