

Supporting Information

Surface-Dependent Activation of Model α -Al₂O₃-Supported P-Doped Hydrotreating Catalysts Prepared by Spin Coating

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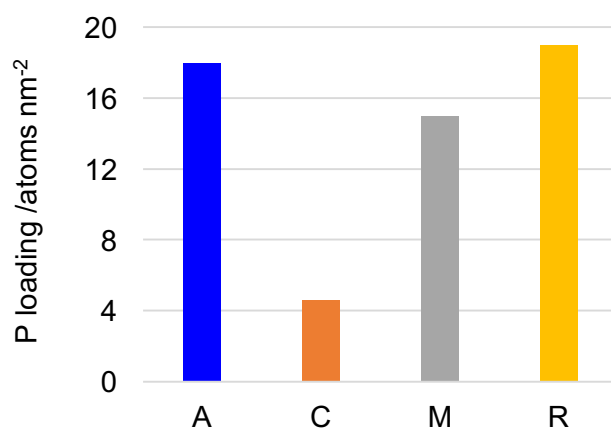


Figure S.1. Surface phosphorus densities obtained with XPS on the A($11\bar{2}0$), C(0001), M($10\bar{1}0$) and R($1\bar{1}02$) crystal planes of α -Al₂O₃ after spin-coating deposition of a phosphate solution. The samples were analyzed after calcination at 450 °C.

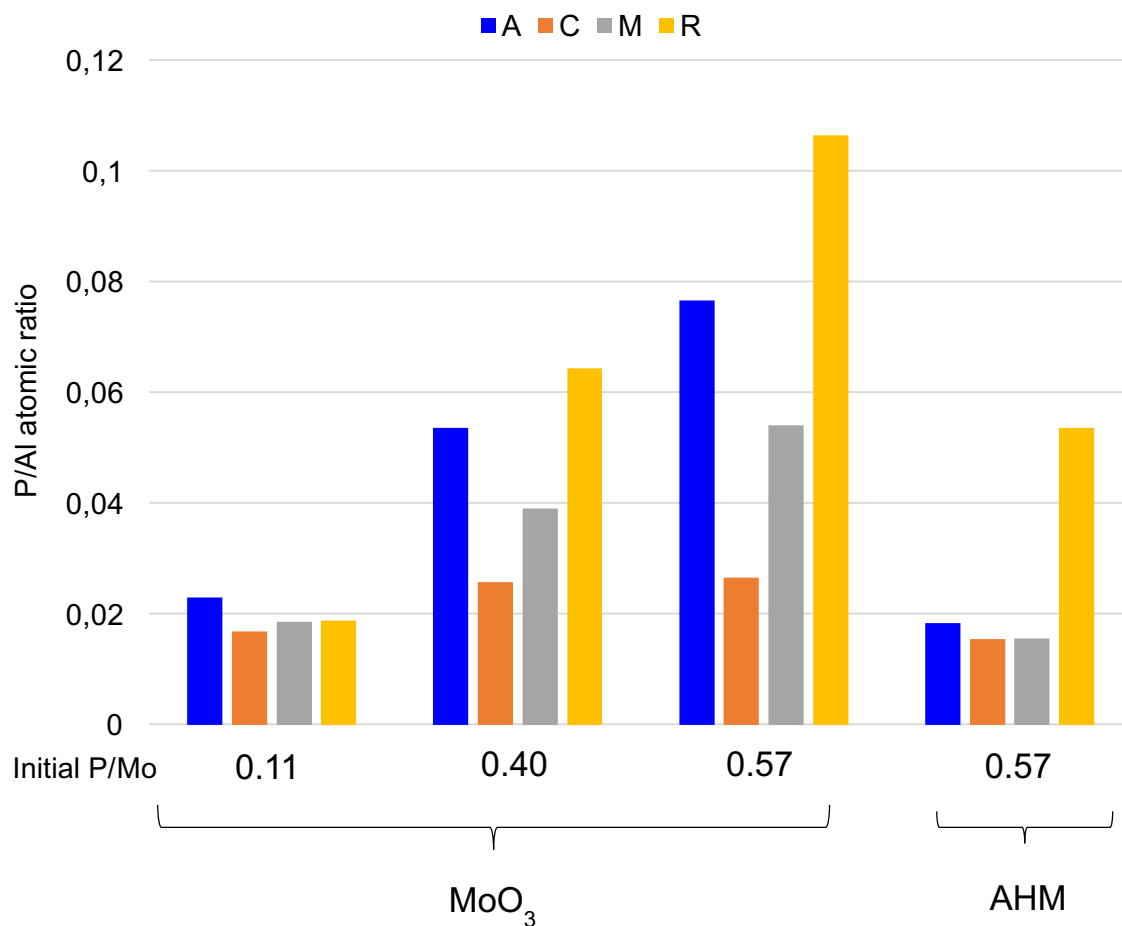


Figure S.2. P/Al atomic ratio for model Mo-P HDS catalysts supported on the A(11 $\bar{2}$ 0), C(0001), M(10 $\bar{1}$ 0) and R(1 $\bar{1}$ 02) crystal planes of α -Al₂O₃ prepared by spin-coating in the oxide phase (after 450 °C/2h calcination) for different precursor solutions (MoO₃ or AHM-based) and varying initial P/Mo in solution

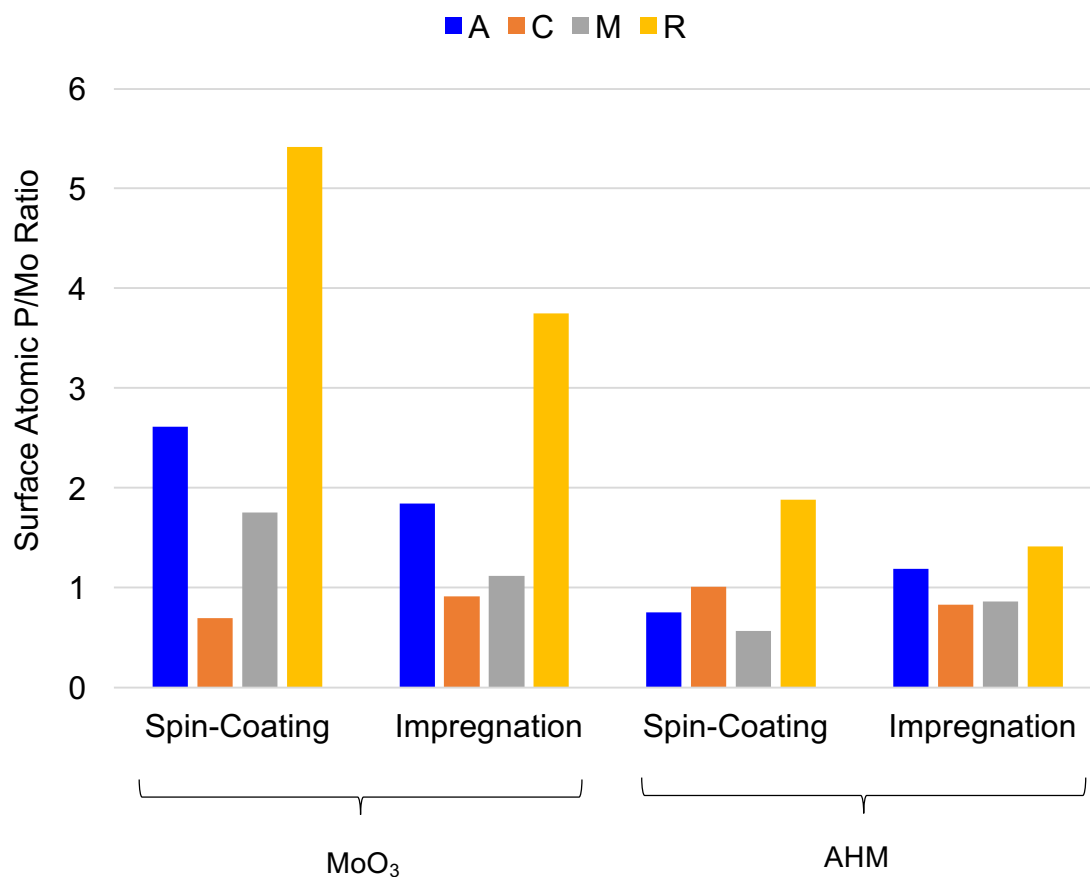


Figure S.3. Comparison of XPS quantification of P/Mo surface atomic ratio for impregnation and spin-coating-synthesized model catalysts in oxide state (calcined at 450°C/2h) for different precursors solutions (MoO₃ or AHM based) with initial P/Mo ratio in solution = 0.57, supported on the A(11 $\bar{2}$ 0), C(0001), M(10 $\bar{1}$ 0) and R(1 $\bar{1}$ 02) crystal planes of α -Al₂O₃.

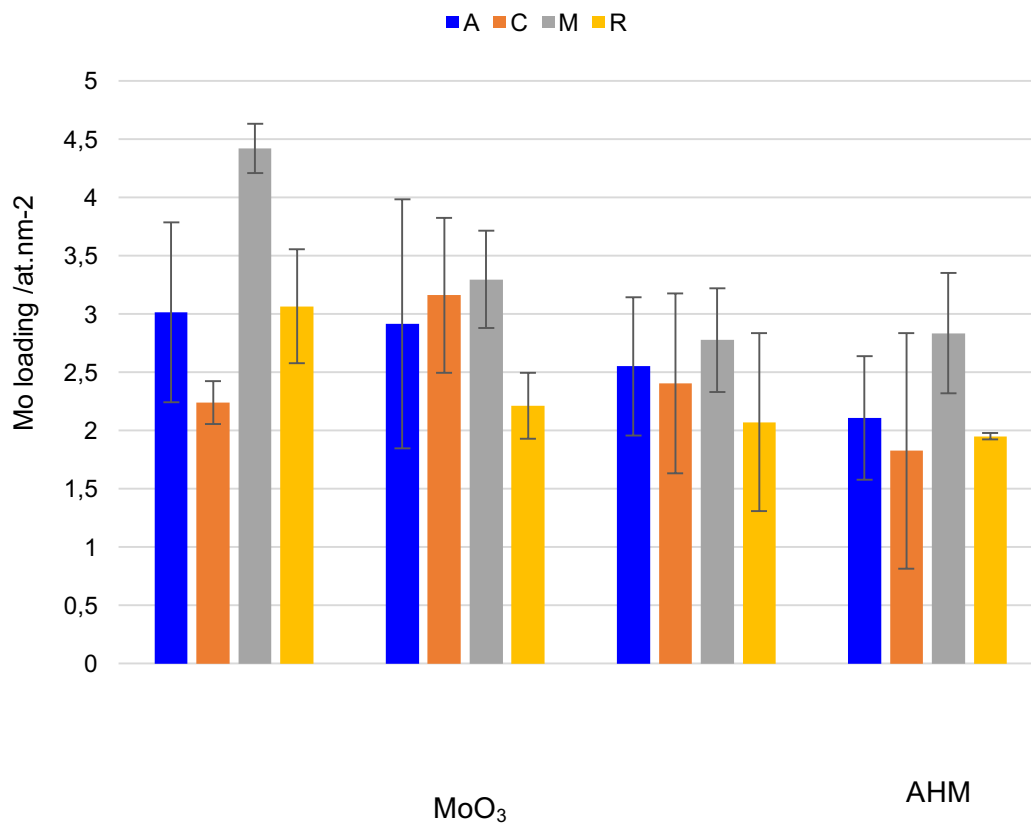


Figure S.4. Average molybdenum loadings (2-3 samples each) obtained by XPS for the model Mo-P/ α -Al₂O₃ catalysts in oxide state (calcined at 450°C/2h) for different precursor solutions (MoO₃ or AHM) with varying initial P/Mo ratio, supported on the A(11 $\bar{2}$ 0), C(0001), M(10 $\bar{1}$ 0) and R(1 $\bar{1}$ 02) α -Al₂O₃ crystal planes. Error bars give the standard deviation obtained on 2-3 samples

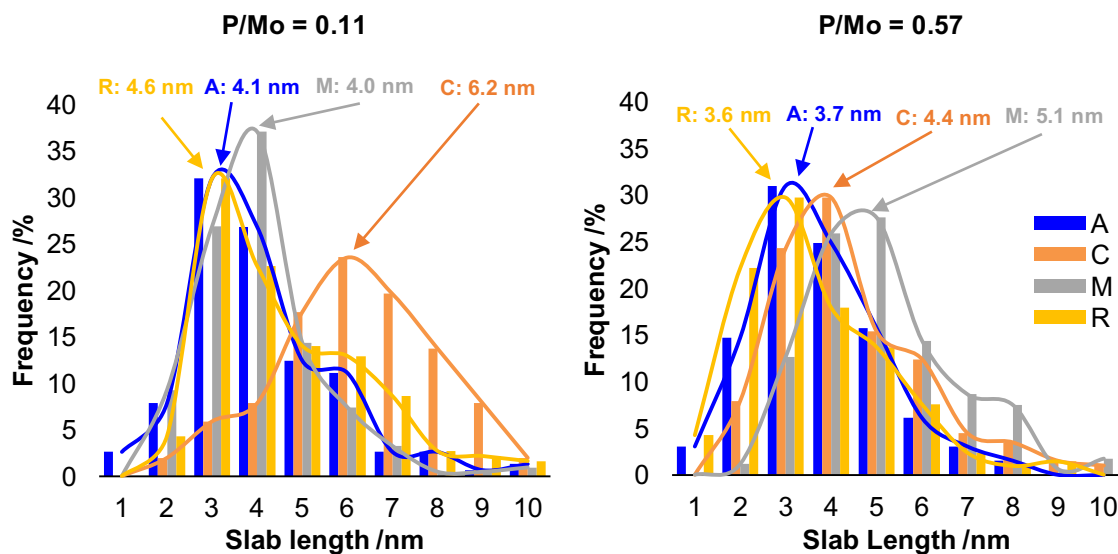


Figure S.5. MoS₂ slab length for model P-doped MoS₂ catalysts supported on the C(0001), A(11 $\bar{2}$ 0), M(10 $\bar{1}$ 0) and R(1 $\bar{1}$ 02) planes of α -Al₂O₃, prepared with the P/Mo = 0.11 (left) and P/Mo = 0.57 (right) precursor solution from MoO₃, sulfided at 400 °C. Surface P/Mo for planes C(0001), A(11 $\bar{2}$ 0), M(10 $\bar{1}$ 0) and R(1 $\bar{1}$ 02) are 0.9, 0.3, 0.3 and 0.7 for the P/Mo=0.11 solution respectively. Surface P/Mo for planes C(0001), A(11 $\bar{2}$ 0), M(10 $\bar{1}$ 0) and R(1 $\bar{1}$ 02) are 2.6, 0.7, 1.8 and 5.4 for the P/Mo=0.57 solution respectively

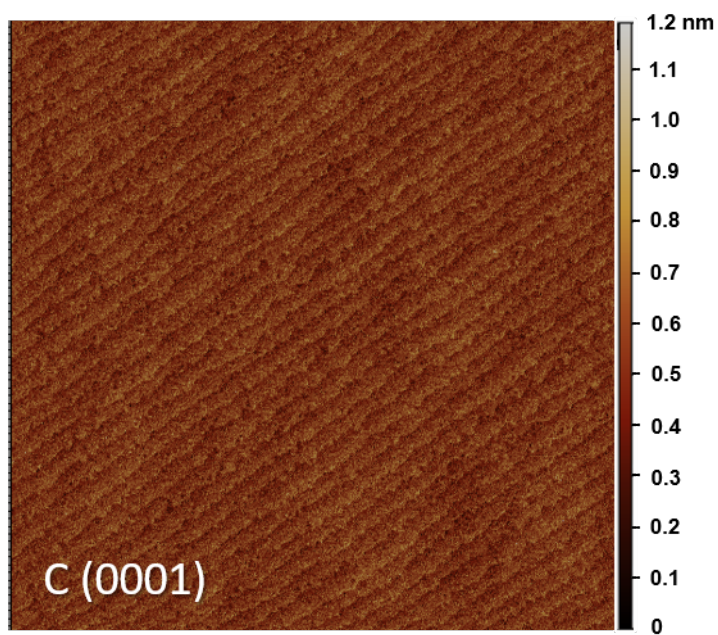
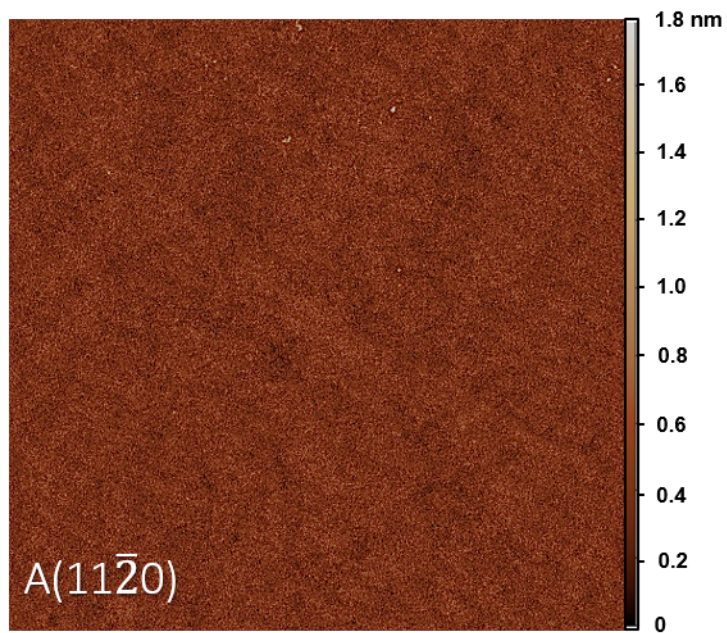


Figure S.6. 2 μm x 2 μm AFM images of the A(11 $\bar{2}$ 0) and C(0001) crystal planes of $\alpha\text{-Al}_2\text{O}_3$ after chemical cleaning with HNO_3 and NH_4OH and calcination at 700 $^\circ\text{C}$ with their height scale in the z-axis.

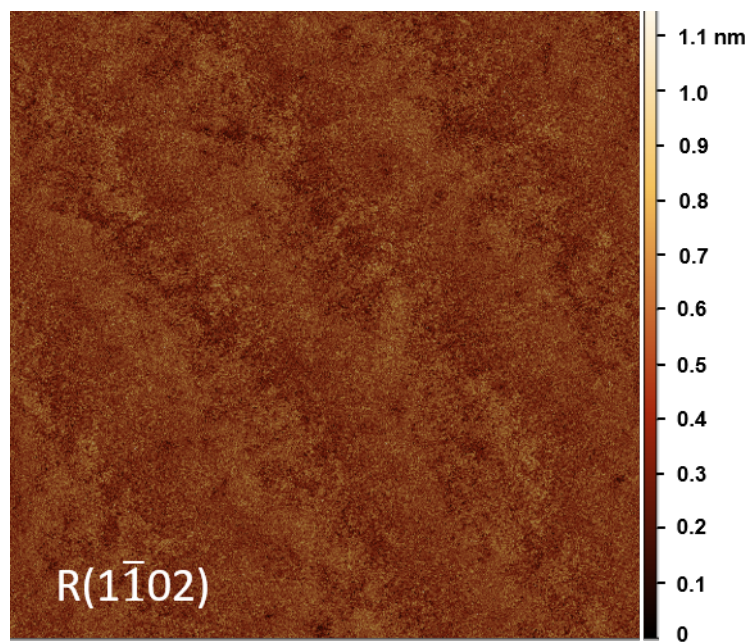
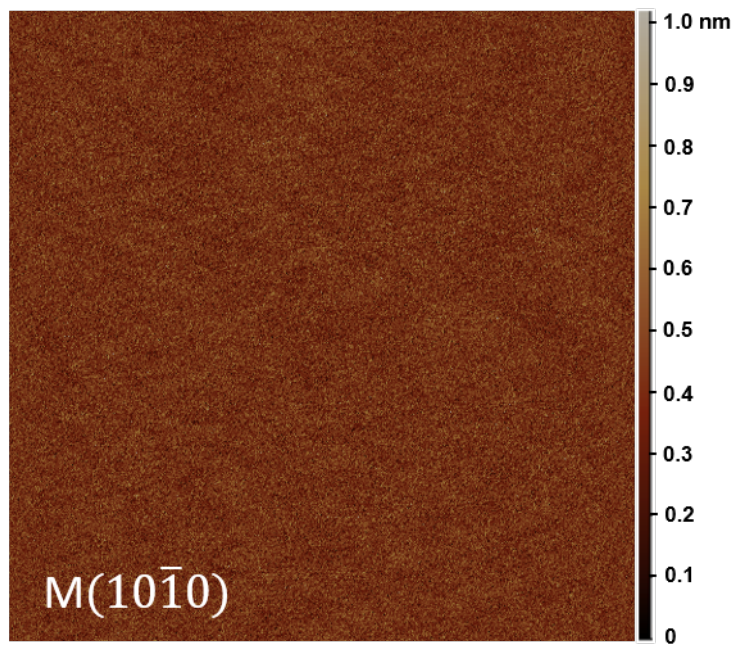


Figure S.7. 2 μm x 2 μm AFM images of the M(10 $\bar{1}$ 0) and R(1 $\bar{1}$ 02) crystal planes of $\alpha\text{-Al}_2\text{O}_3$ after chemical cleaning with HNO_3 and NH_4OH and calcination at 700 $^\circ\text{C}$ with their height scale in the z-axis.