Supporting Information

Effect of oxygen vacancies and crystal phases in defective Pt/ZrO_{2-x} on its photocatalytic activity toward hydrogen production

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Table S1. Lattice parameters of the models for DFT calculation.

system	*a*	*b*	*c*	α	β	γ
Monoclinic (111) slab	7.3207	7.4378	15.2518	90	90	114.68
Tetragonal (101) slab	6.4049	3.6400	19.9195	90	90	90

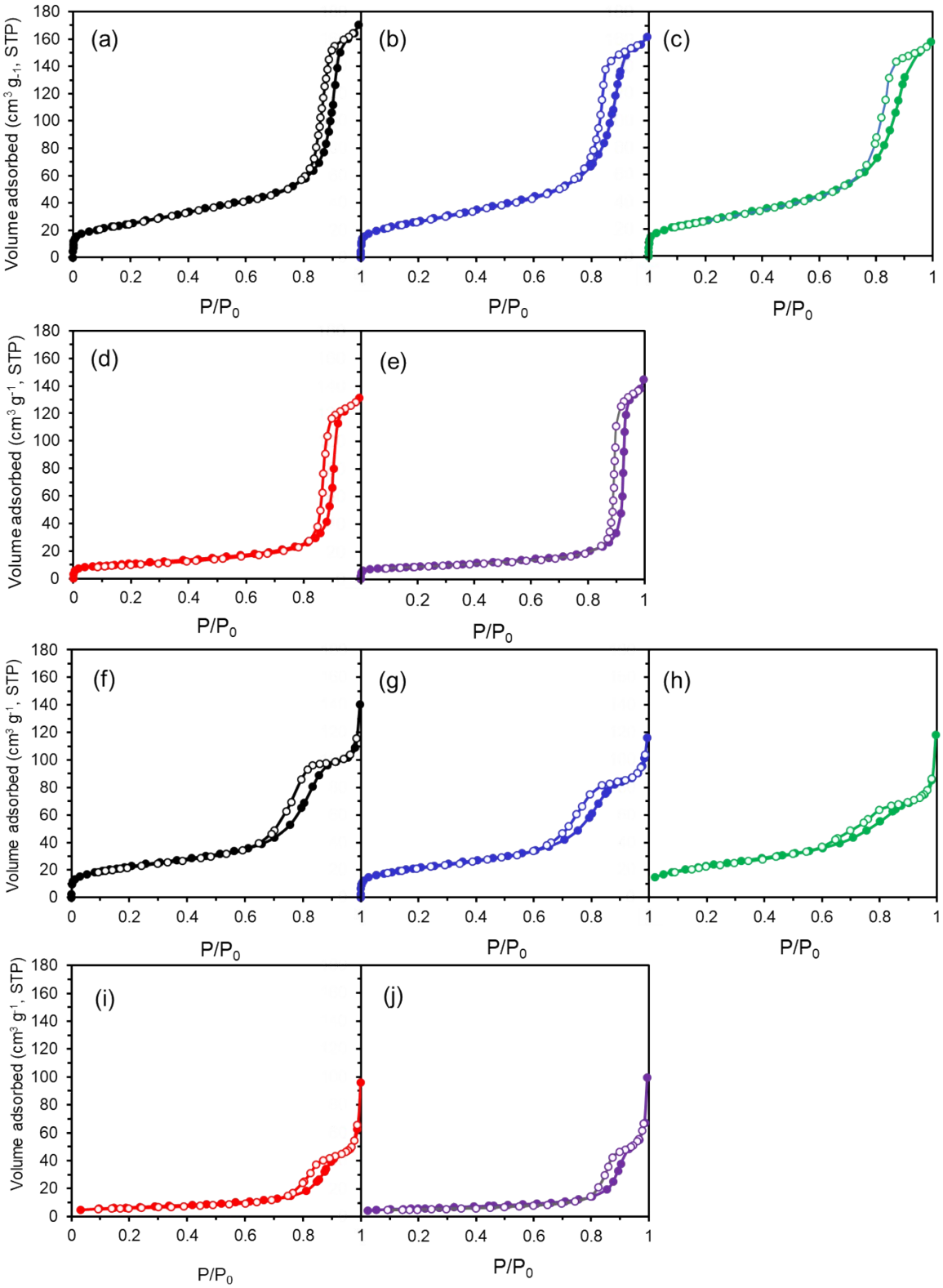

Figure S1. N_2 adsorption/desorption isotherms of (a) as-synthesized *m*-ZrO_2, (b) Pt/*m*-ZrO_{2-x}200, (c) Pt/*m*-ZrO_{2-x}400, (d) Pt/*m*-ZrO_{2-x}600, (e) Pt/*m*-ZrO_{2-x}600_6h, (f) as-synthesized *t*-ZrO_2, (g) Pt/*t*-ZrO_{2-x}200, (h) Pt/*t*-ZrO_{2-x}400, (i) Pt/*t*-ZrO_{2-x}600, and (j) Pt/*t*-ZrO_{2-x}600_6h.

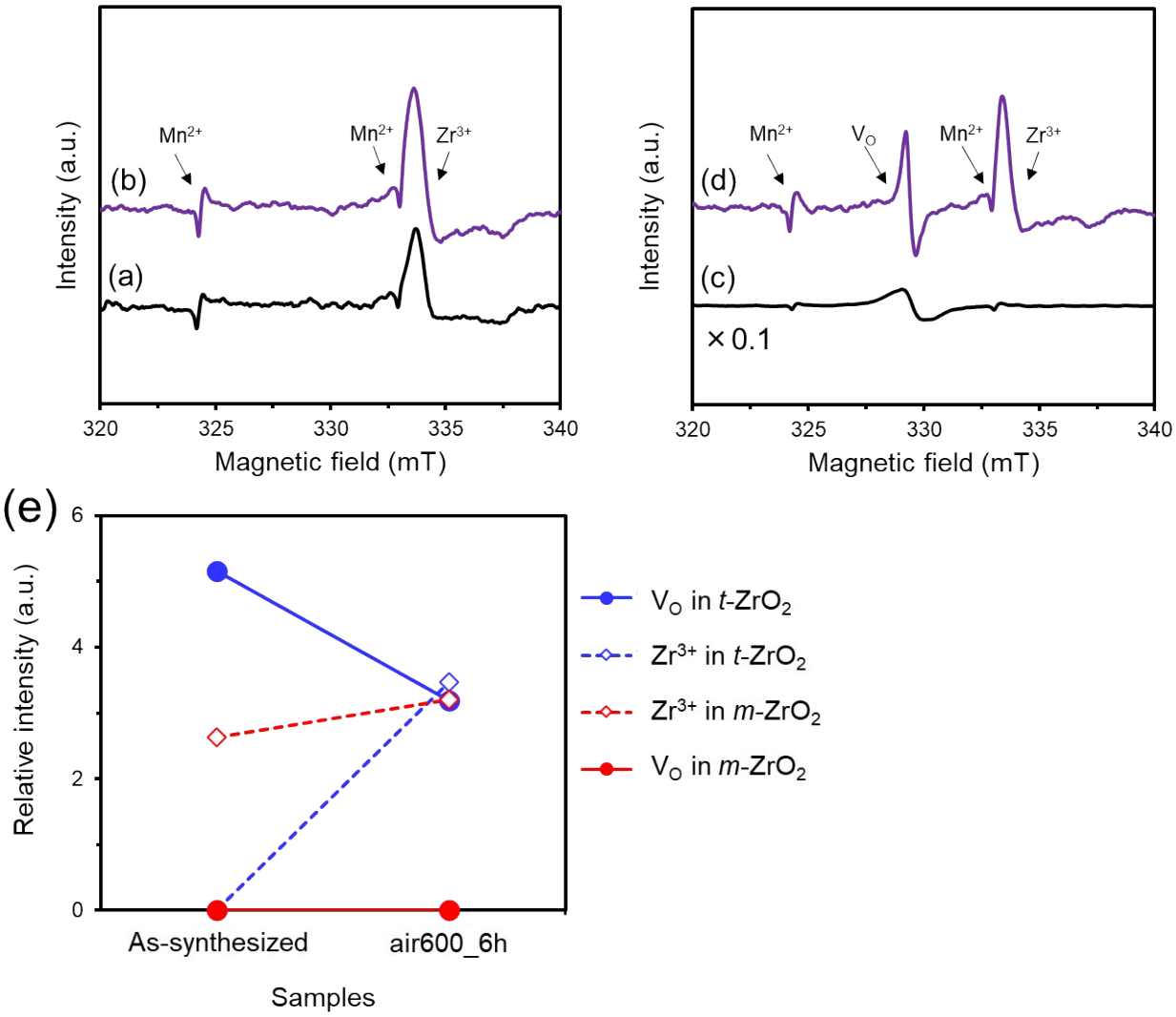

Figure S2. ESR spectra of (a) as-synthesized *m*-ZrO_2, (b) *m*-ZrO_2 after calcination, (c) as-synthesized *t*-ZrO_2, and (d) *t*-ZrO_2 after calcination at 600 °C for 6 h. (e) Relative intensity of the ESR signals based on Mn^{2+}.

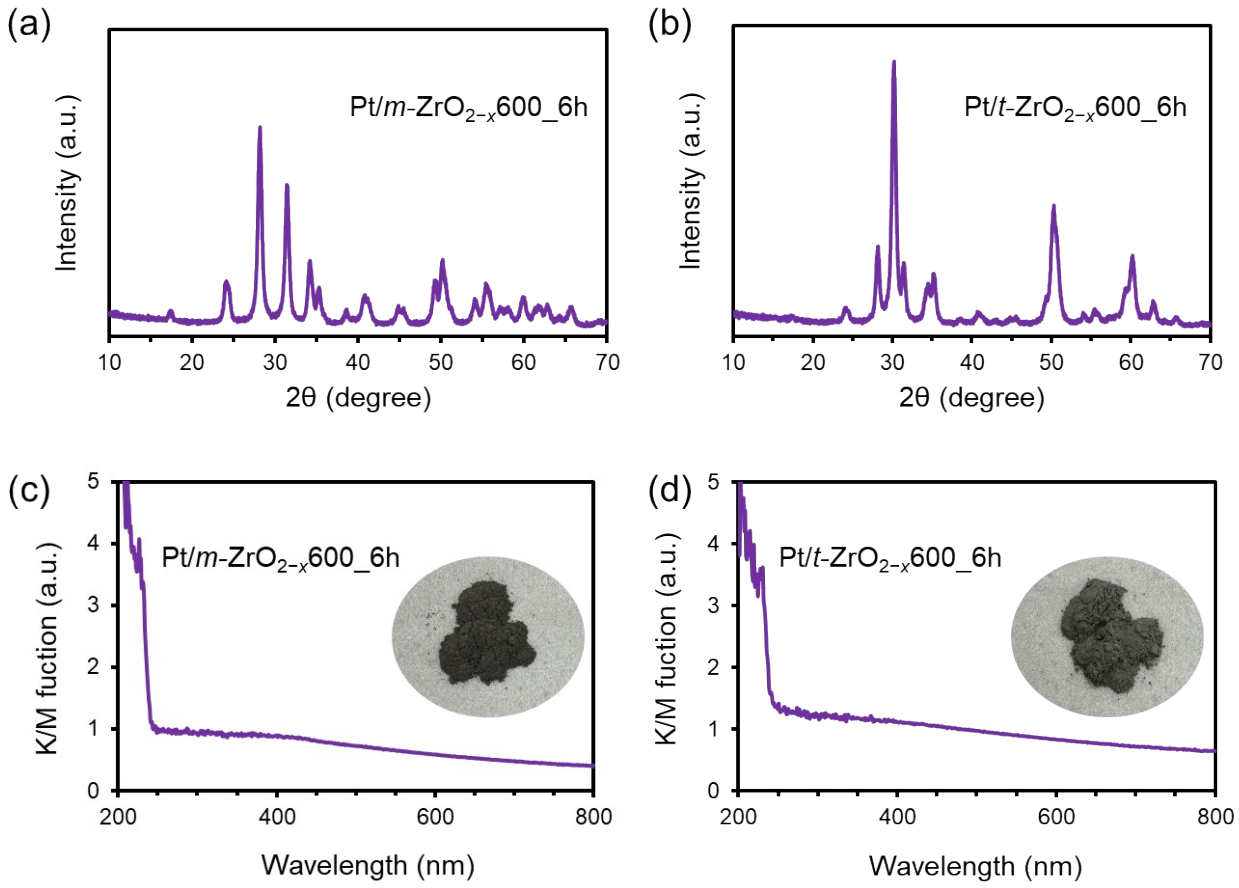

Figure S3. XRD patterns of (a) Pt/*m*-ZrO_{2-x}600_6h and (b) Pt/*t*-ZrO_{2-x}600_6h. Diffuse-reflectance spectra and photographs of (c) Pt/*m*-ZrO_{2-x}600_6h and (d) Pt/*t*-ZrO_{2-x}600_6h.

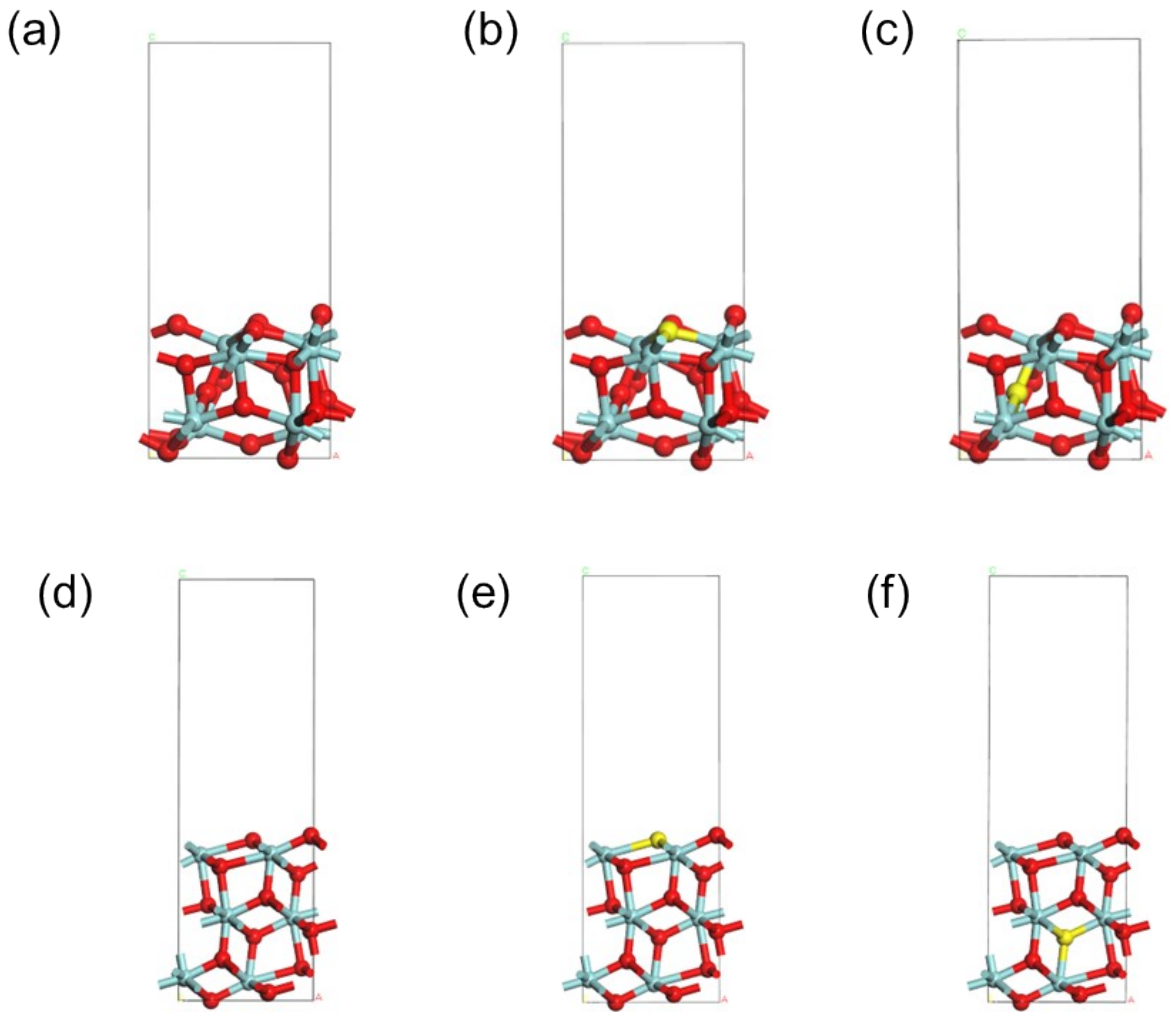

Figure S4. Models of monoclinic ZrO_2 (111) with (a) no defect, (b) a surface V_O, (c) a bulk V_O, and tetragonal ZrO_2 (101) with (d) no defect, (e) a surface V_O, (f) a bulk V_O. Red and blue balls display O and Zr atom, respectively. Yellow balls are O atoms removed to form V_O prior to the calculation.