

Supporting Information:

Enhanced performance of oxygen vacancies on the CO₂ adsorption and activation over different phases of ZrO₂

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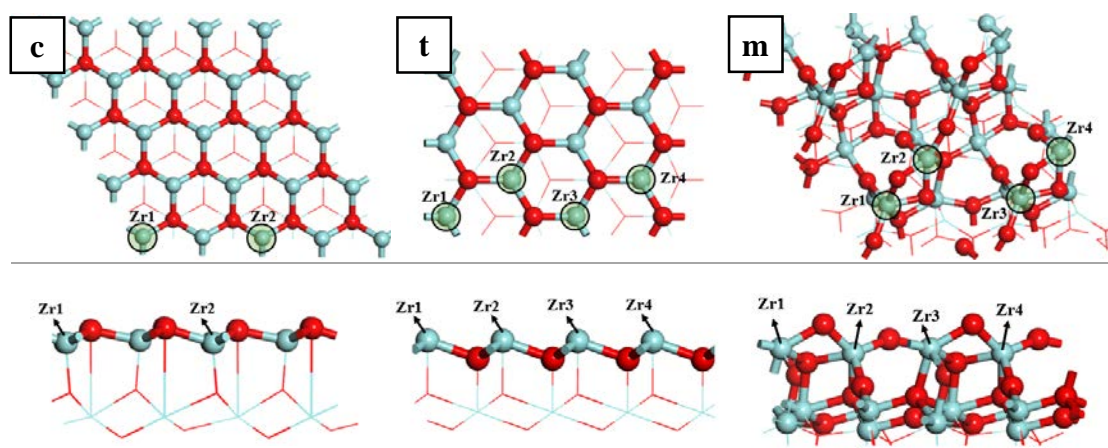


Figure S1 Optimized perfect ZrO₂ surface. (O atoms in red, Zr atoms in blue, green circles are highlighted symbols.)

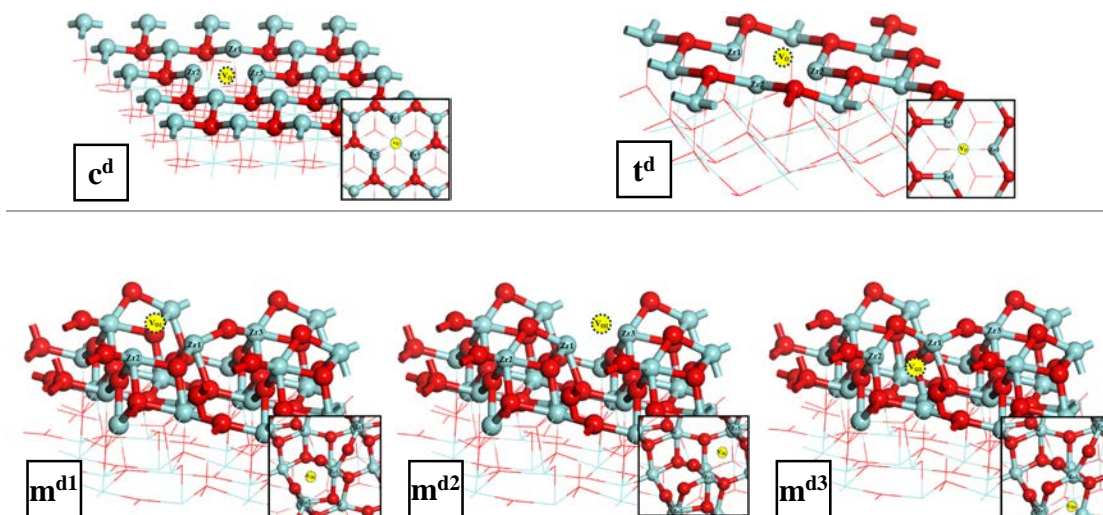


Figure S2 ZrO₂ surface with oxygen vacancies. (The large figure is a side view and the box view is a top view, and oxygen vacancy marked by yellow.)