Electronic Supplementary Information

Mechanism and activity of oxygen reduction reaction on WTe_2 transition metal dichalcogenide with Te vacancy

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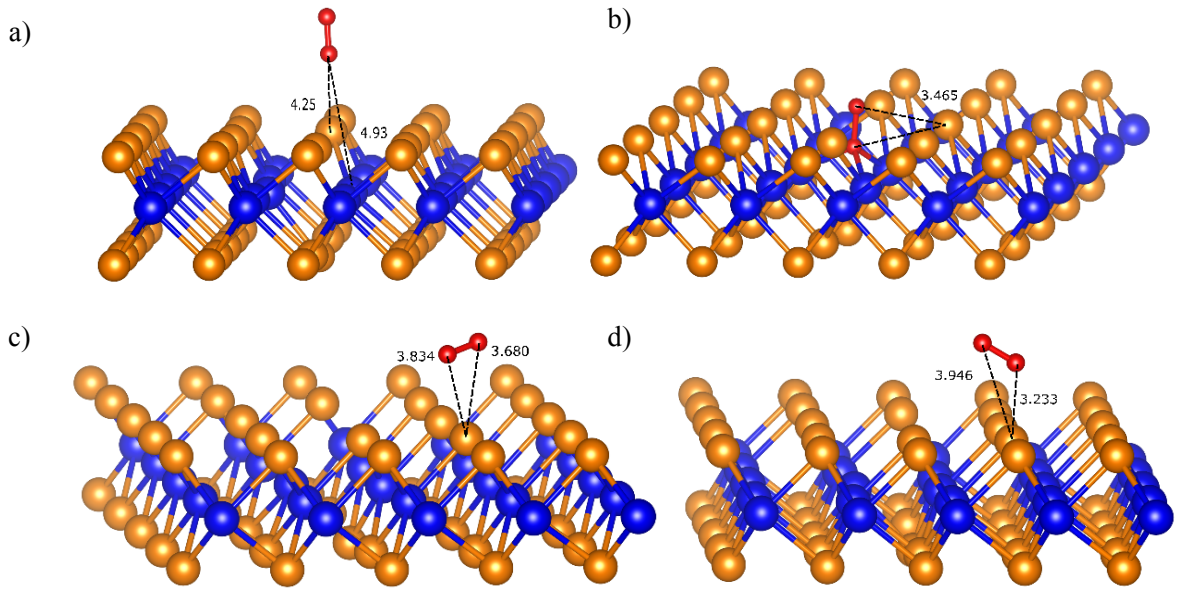

Figure S1. The favorable structures of the molecular oxygen adsorption on WTe_2^d: D3 in region I (a), D4 in region II (b), P2 in region III (c), and P3 in region III (d). Where the name of each configuration is enclosed with letter D and P for defect and perfect regions, respectively. The color spheres: W – blue, Te – orange, and O – red.