

Hydration mechanisms of tungsten trioxide revealed by water adsorption isotherms and first-principles molecular dynamics simulations: Supporting Information

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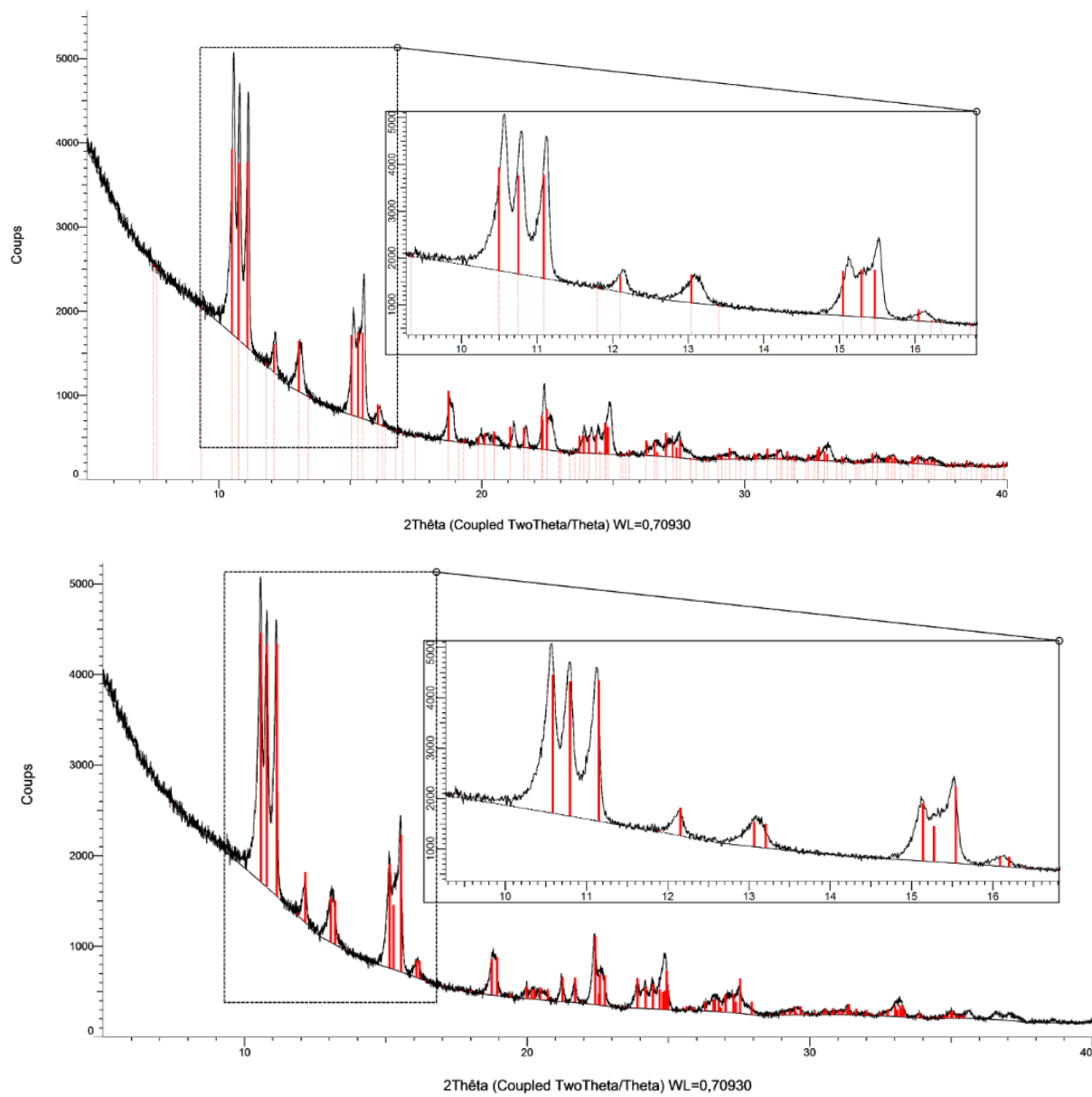


Figure S1. Fits of the XRD spectrum with: a) orthorhombic; and b) cubic WO_3 phases.

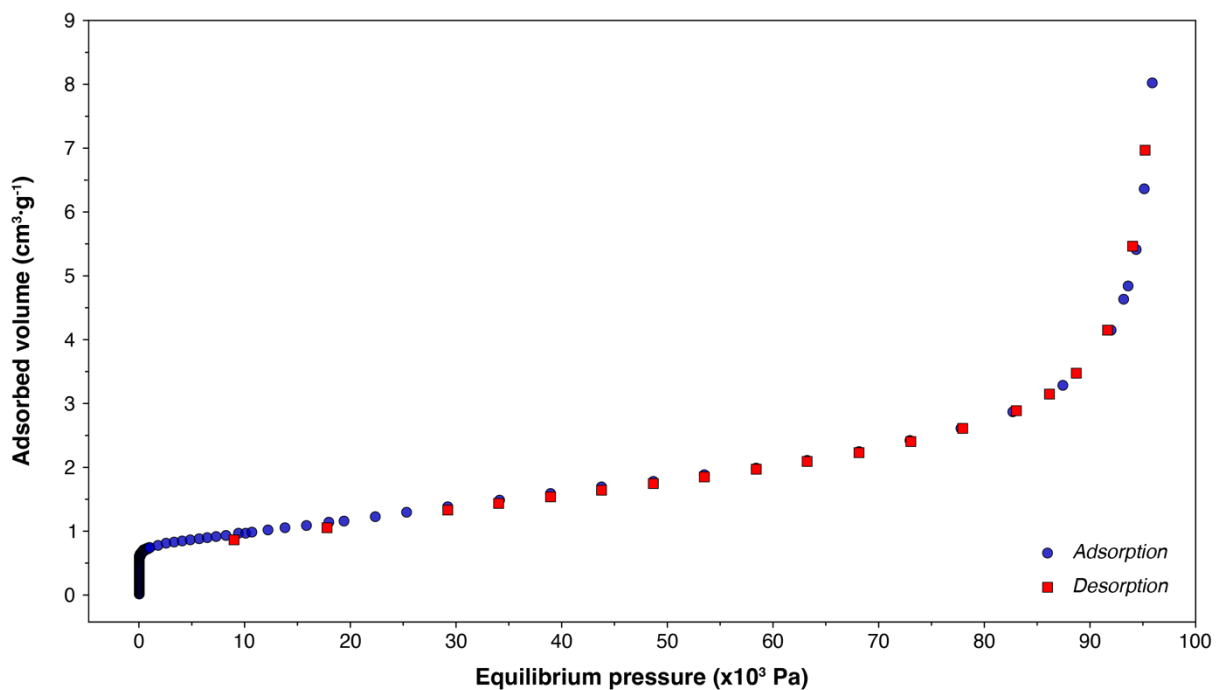


Figure S2. Adsorption and desorption branches of N₂ at 77K on the synthesized WO₃ powder.

Table S1. Calculated adsorption energies in vacuum (including implicit solvent), dispersion energies and isosteric adsorption energies, at 0 K, as a function of explicit water coverage.

n (number of H ₂ O)	$\Delta E_{\text{ads}/\text{H}_2\text{O}}$ (kJ·mol ⁻¹)	$\Delta E_{\text{disp}/\text{H}_2\text{O}}$ (kJ·mol ⁻¹)	$\Delta E_{\text{ads}}^{\text{iso}}$ (kJ·mol ⁻¹)
1	-107.3 (-64.4)	-22.7	
2	-107.7 (-65.3)	-25.5	-108.2
4	-106.2 (-65.1)	-26.4	-104.7
6	-105.6 (-65.3)	-27.1	-104.5
7	-105.2 (-65.2)	-27.3	-102.5
8	-104.9 (-64.6)	-27.1	-103.0
9	-99.5 (-62.6)	-25.1	-56.2
10	-95.9 (-59.4)	-24.4	-63.6
12	-92.4 (-57.4)	-22.6	-74.5

14	-87.8 (-54.4)	-21.1	-60.7
16	-86.6 (-53.5)	-19.8	-77.7
18	-83.8 (-50.4)	-19.6	-61.4
20	-80.9 (-48.5)	-19.1	-55.0
21	-80.0 (-47.3)	-19.1	-61.0
22	-79.2 (-46.8)	-19.0	-63.1
24	-77.5 (-45.6)	-17.5	-58.7
26	-77.0 (-45.5)	-16.9	-71.8
28	-76.5 (-44.8)	-16.5	-69.9
30	-76.0 (-45.3)	-16.3	-69.1
32	-76.0 (-45.6)	-15.8	-75.9

Internal coordinates of the full hydrated WO₃ model

a1, a2, a3: 14.8854799999999994 0.0000000000000000 0.0000000000000000
b1, b2, b3: 0.0000000000000000 15.1516000000000000 0.0000000000000000
c1, c2, c3: -0.7530670907407410 0.0000000000000000 33.0000000000000000

Atom types: H O W O

Atom numbers: 320 160 48 144

Internal coordinates:

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