Supplementary Material for: "Water Oxidizes The Surface of Ultrasmall 4 Å Single-walled Carbon Nanotubes and fullerene C20"

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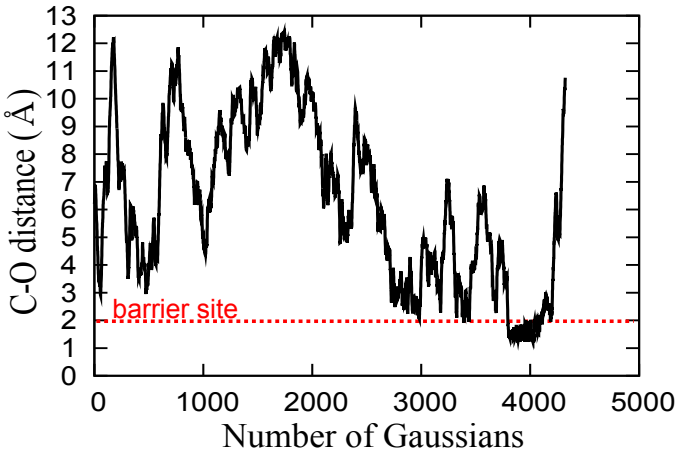

FIG. S1. Evolution of the coordination number (ξ) with respect to the number of Gaussian functions (N_G) for V^{3+}(aq).

I. METADYNAMIC SIMULATIONS

Figure S1 shows the evolution of bond distance between the oxygen atom of water molecule and one of the C atoms on the surface of 4 Å SWCNT tube (5,0), as a function of the number of Gaussians N_G used to reconstruct the free energy profile for the water first dissociation reaction on the surface of tube (5,0) in Figure 3 (a). In this Figure S1, the selected H_2O was diffusing in the aqueous solution with the collective variable ranging from 12.6 to 2.0 Å. The activation energy barrier is picked when the bond distance = 2.0 Å which corresponds to when the number of Gaussians = 3780. The water dissociation reaction is complete after addition of 4200 number of Gaussians. The reconstruction of free energy profile in Figure 3(a) is based on the results at 4200 Gaussians.

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