Supporting Information

Molecular Dynamics Study on the Adsorption of UO_2^{2+} from an Aqueous Phase: Effect of Grafting Dibenzo Crown Ether and Dicyclohexano Crown Ether on the Polystyrene surface.

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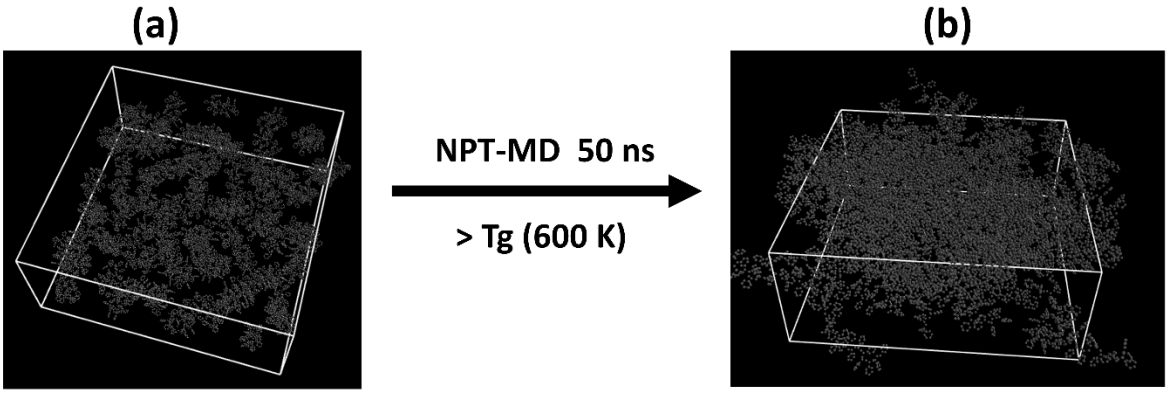

Figure S1. Aggregation of PS chain with increase in temperature greater than Tg. (a) Initial chain distribution, (b) random aggregation of PS chains.

In the first step, we created an amorphous polymer surface equivalent to the experimental density .[1] To that end, we performed a simulation of 20 repeat unit of single PS chain in water in a 8 nm cubic box, 100 ps NVT and 100 ps NPT simulations followed by 20 ns NPT-MD simulations using the periodic boundary conditions in the x, y and z directions. The equilibrated chain is used for the generation of multiple polymer chains, by placing the chains, 50 in number, randomly in the box of 12×12×9 nm in size. Subsequently, we have performed NPT-MD simulation for 50 ns at a temperature of 600 K using periodic boundary conditions in all the directions. The simulation snapshot of PS aggregation is presented in Figure S1 of the supporting information. During the equilibration process the polystyrene chains are found to aggregate to form an amorphous polymer melt after equilibration. The box dimension for this amorphous polymer sample is enlarged for 20 nm in the z-direction to provide a vacuum slab on top of the aggregated polymeric surface. The NVT-MD simulations are performed for this enlarged system for another 20 ns in order to generate the smooth polymer surface as shown in Figure 1. We observed that 20 ns run is sufficient for the density of 0.911 g/cm^3, similar to the experimental density of 0.914 g/cm^3.[1] This procedure is similar to the method adopted in the literature.[2] After the equilibration, the temperature of the simulated system is cooled to a temperature of 300 K at the rate of 0.01 K/ps. The final amorphous surface has the thickness of approximately ~4 nm, the final box dimensions of the surface as 7.06×7.06×3.7 nm.

1. Zoller, P.; Walsh, D. J. In Standard Pressure-Volume-Temperature Data for Polymers; Technomic: Lancaster, 1995; p 412.
2. Selemon, B.; Tsige, M. Interfacial properties of oxidized polystyrene and its interaction with water. *Langmuir* **2013**, *29*, 13230-13238.

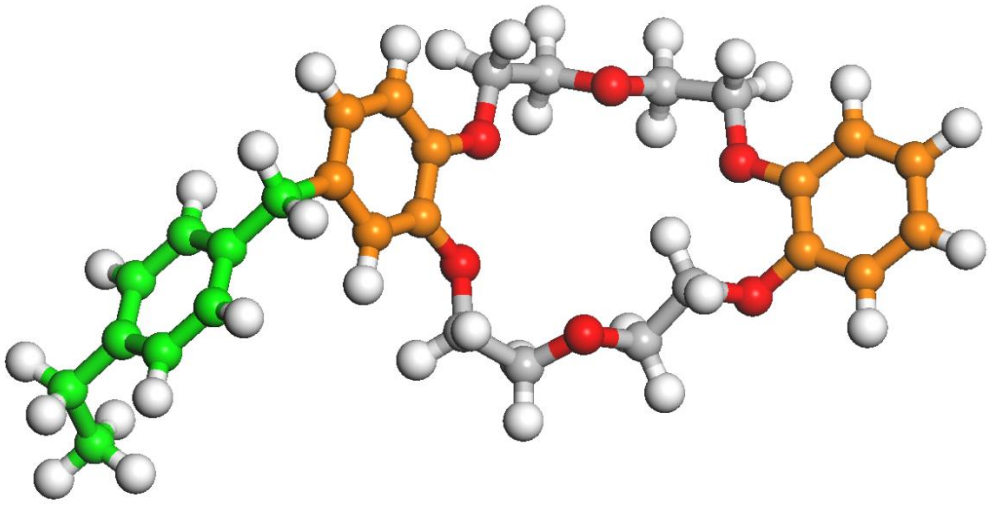

Figure S2. Schematic representation of DBCE grafting on the PS monomer. Green-PS, Gray-Crown-ether and orange-benzene.

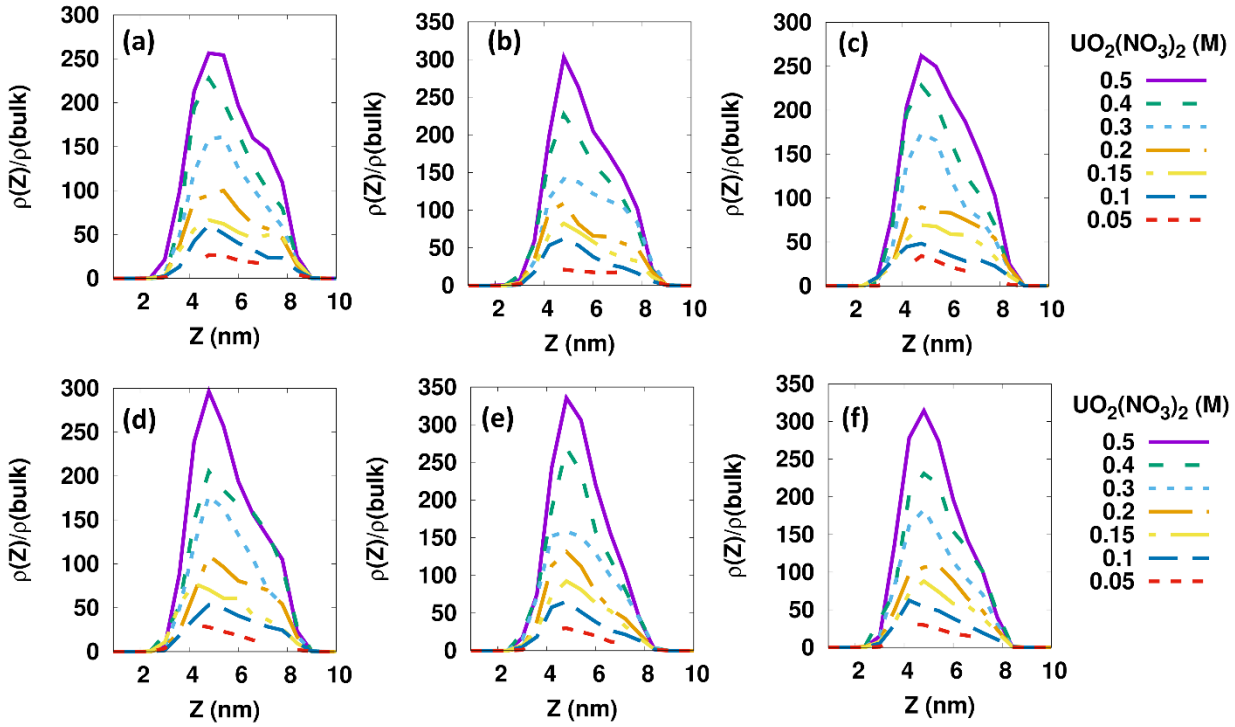

Figure S3. Density distribution of UO_2^{2+} for at DBCE grafting, at grafting density (ρ_s) (a) 0.25, (b) 0.50, (c) 0.75, (d) 1.0, (e) 1.25 and (f) 1.67 mol/nm^2.

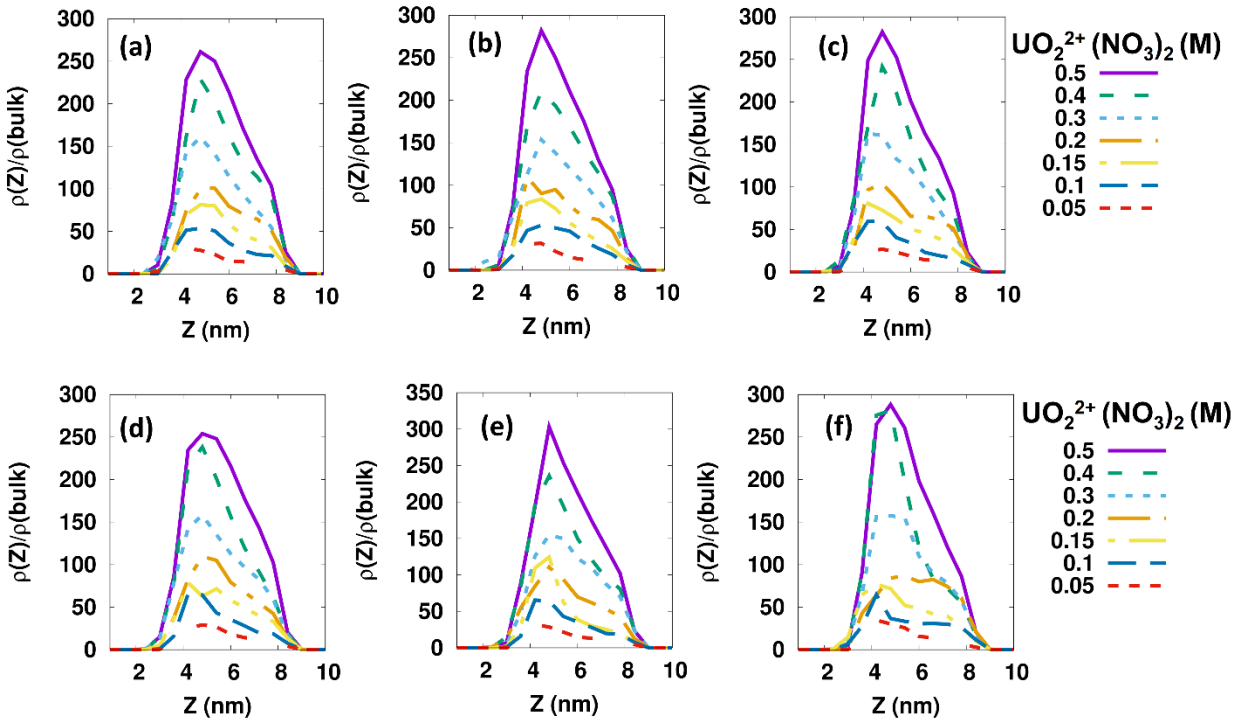

Figure S4. Density distribution of UO_2^{2+} for at DCHCE grafting, at grafting density (ρ_s) (a) 0.25, (b) 0.50, (c) 0.75, (d) 1.0, (e) 1.25 and (f) 1.67 mol/nm^2.

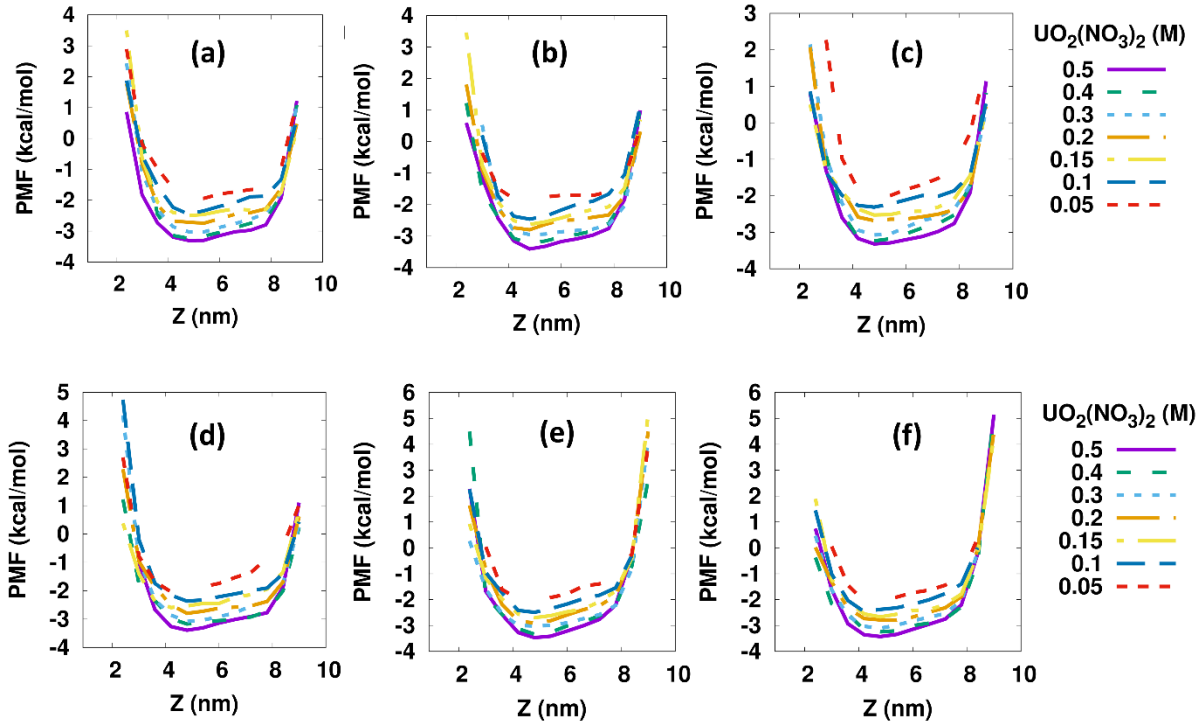

Figure S5. PMF profiles of adsorbed ions of UO_2^{2+} for at DBCE grafting, at grafting density (ρ_s) (a) 0.25, (b) 0.50, (c) 0.75, (d) 1.0, (e) 1.25 and (f) 1.67 mol/nm^2.

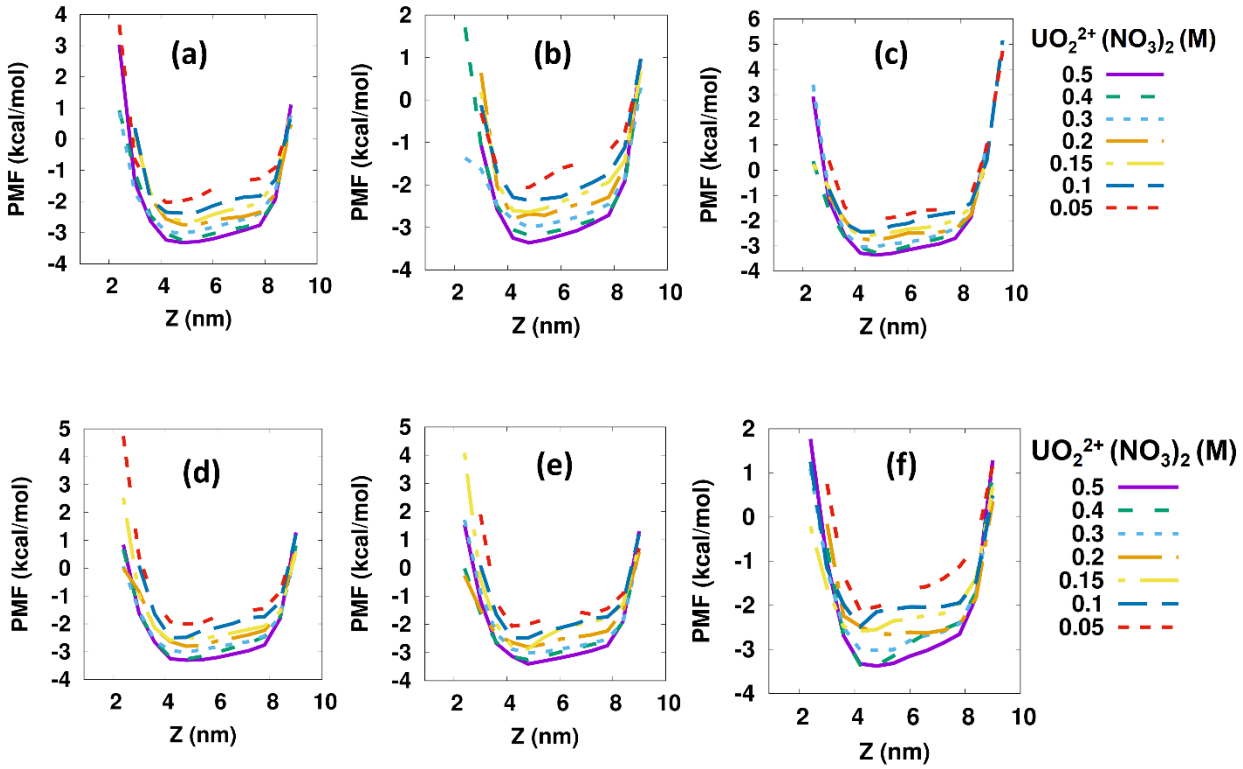

Figure S6. PMF profiles of adsorbed ions of UO_2^{2+} for at DCHCE grafting, at grafting density (ρ_s) (a) 0.25, (b) 0.50, (c) 0.75, (d) 1.0, (e) 1.25 and (f) 1.67 mol/nm^2.