Supplementary Information: Simulations of Graphitic Nanoparticles at Air-Water Interfaces

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Presented in Fig. S1 is the potential mean force or free energy of a single-shell carbon nanoparticle of radius r, transferred through a water layer. The free energy is displayed as a function of contact angle θ and shifted to the energy of the particle in its completely submerged state, $\theta \sim 0°$. For single-shell particles, an energy minimum occurs at $\theta \sim 50°$, corresponding to the energy of the particle at the water-air interface. As the size of the particle grows the energy at the interface deepens. This is particularly notable in the advancing section of the PMF curve (Fig. S1a) and indicates that for single-shell particles, the propensity for adsorption to the air-water interface is enhanced with increasing particle size. Yet based on the position of the energy minimum at the interface, larger single-walled particles exhibit enhanced wetting compared to their smaller analogues. In the case of nano-onions (multi-shell structures), Fig. S2 shows that the minimum at the air-water interface is replaced by a saddle point, suggesting that these multi-walled particles are significantly less surface active.

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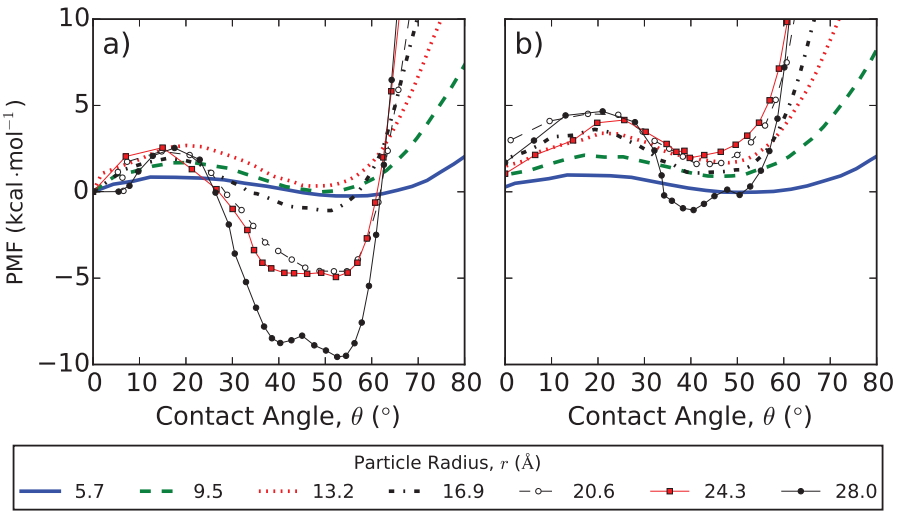

Figure S1: Free energy curve obtained upon a) advancement and b) retraction of single-shell carbon nanoparticles of radius r, through a water layer.

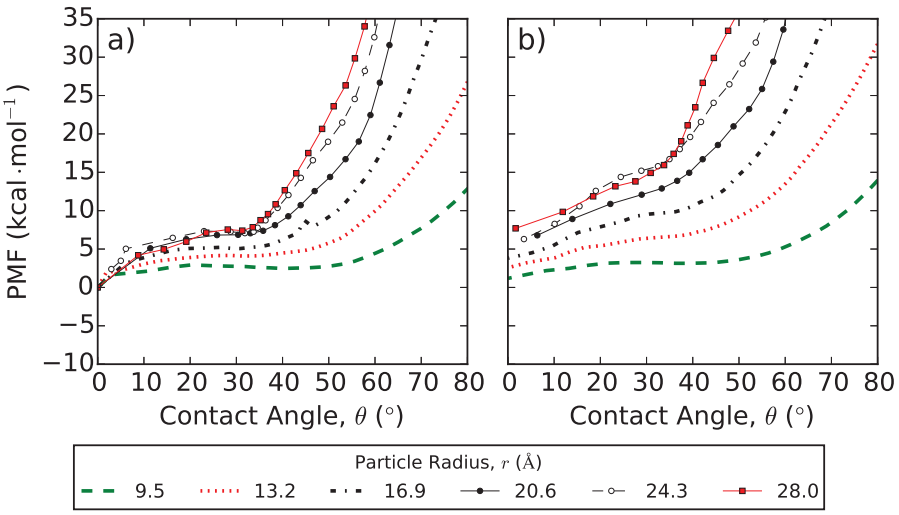

Figure S2: Free energy curve obtained upon a) advancement and b) retraction of multi-shell carbon nanoparticles of radius r, through a water layer.