Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: On the Wetting Translucency of Hexagonal Boron Nitride

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Effect of $\varepsilon_{\mathrm{Au-O}}$ on $U_{\mathrm{CS-W}}$

The parameters obtained from the fit of the computed total potential energy ($U_{\mathrm{CS-W}}$) to a Mie potential (eq. 1 from the main article) are presented in Figure S1 for the substrate coated by monolayer hBN, Figure S2 for a substrate coated by bilayer hBN and Figure S3 for a substrate coated by trilayer hBN. The computed parameters for free standing hBN bilayer are: $n_{\mathrm{hBN-W}} = 9.071$, $m_{\mathrm{hBN-W}} = 4.209$, $\sigma_{\mathrm{hBN-W}} = 2.815$ Å, and $\varepsilon_{\mathrm{hBN-W}} = 1.985$ kcal/mol. The computed parameters for free standing hBN trilayer are: $n_{\mathrm{hBN-W}} = 9.121$, $m_{\mathrm{hBN-W}} = 4.148$, $\sigma_{\mathrm{hBN-W}} = 2.812$ Å, and $\varepsilon_{\mathrm{hBN-W}} = 2.012$ kcal/mol.

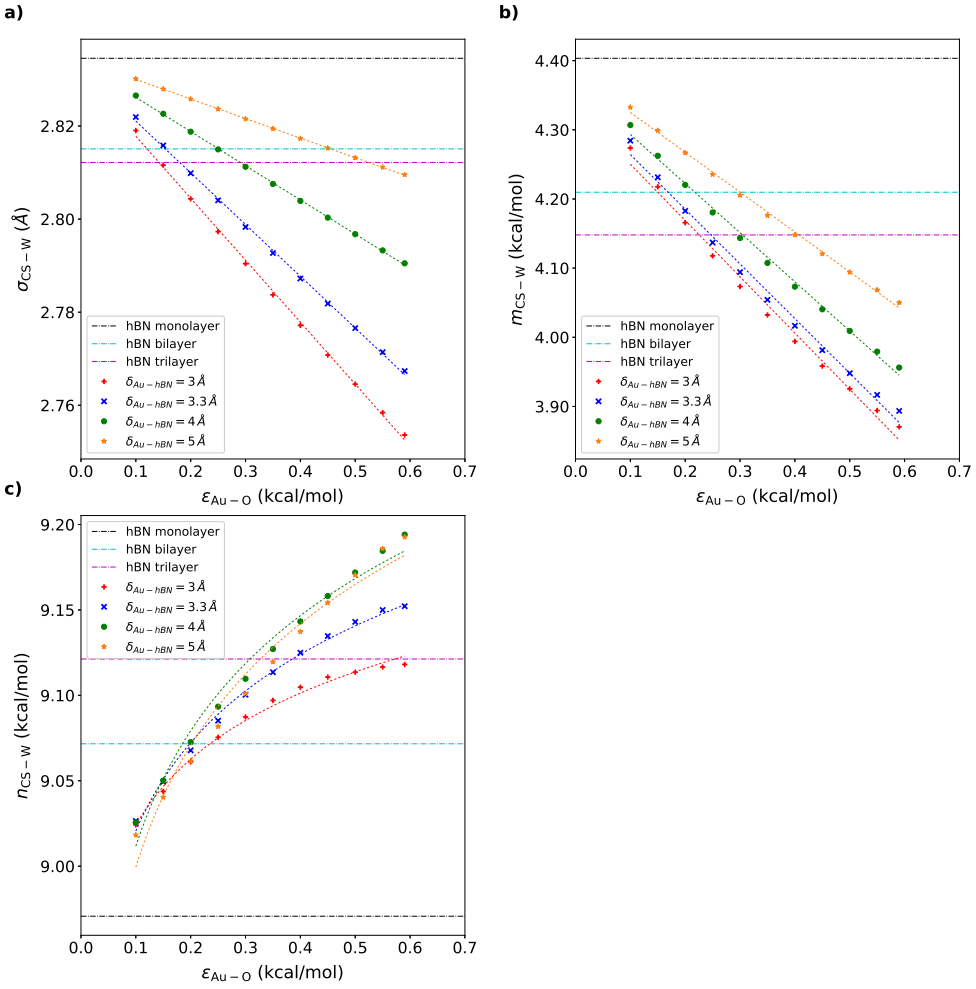

Figure S1: Parameters for the coated substrate-water interaction, obtained from the fit to a Mie potential (eq. 1 from the main article). The computed parameters correspond to a surface coated by a monolayer hBN, with different contact distances ($\delta_{\mathrm{Au-hBN}}$). a) $\sigma_{\mathrm{CS-W}}$. b) $m_{\mathrm{CS-W}}$. c) $n_{\mathrm{CS-W}}$.

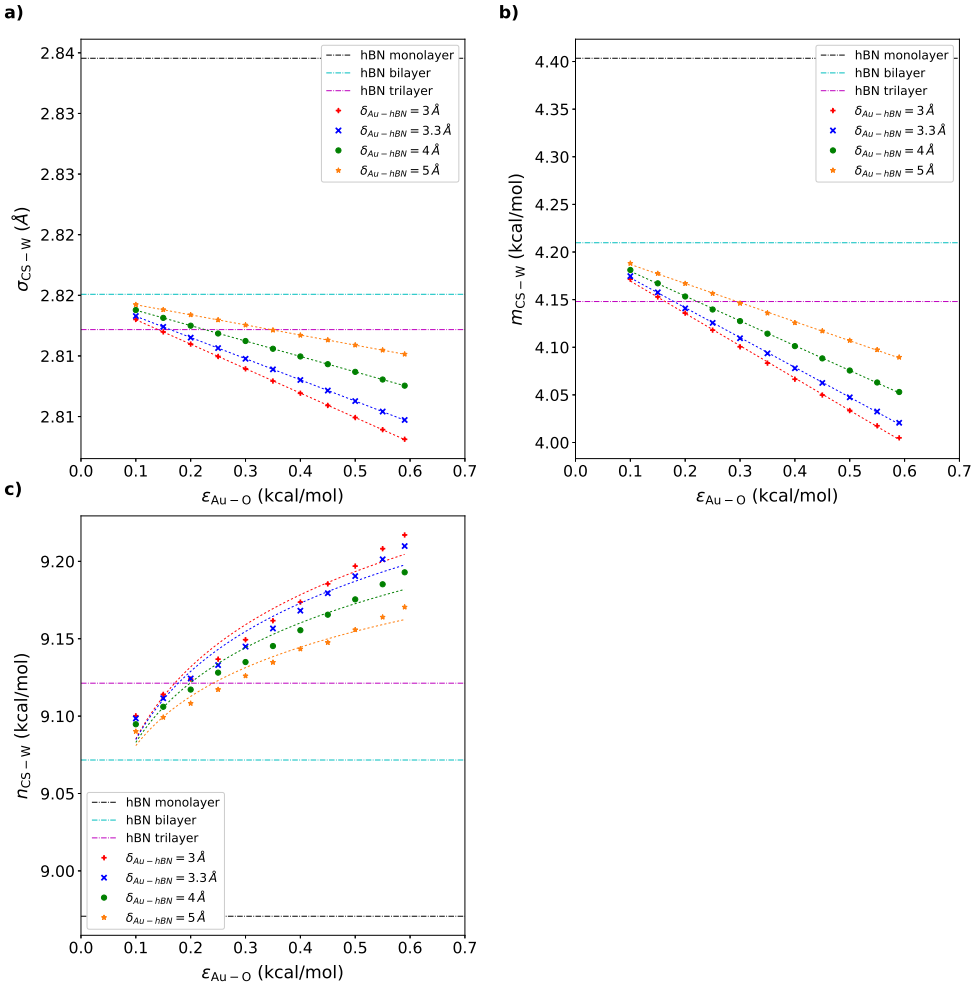

Figure S2: Parameters for the coated substrate-water interaction, obtained from the fit to a Mie potential (eq. 1 from the main article). The computed parameters correspond to a surface coated by bilayer hBN, with different contact distances ($\delta_{\mathrm{Au-hBN}}$). a) $\sigma_{\mathrm{CS-W}}$ b) $m_{\mathrm{CS-W}}$ c) $n_{\mathrm{CS-W}}$.

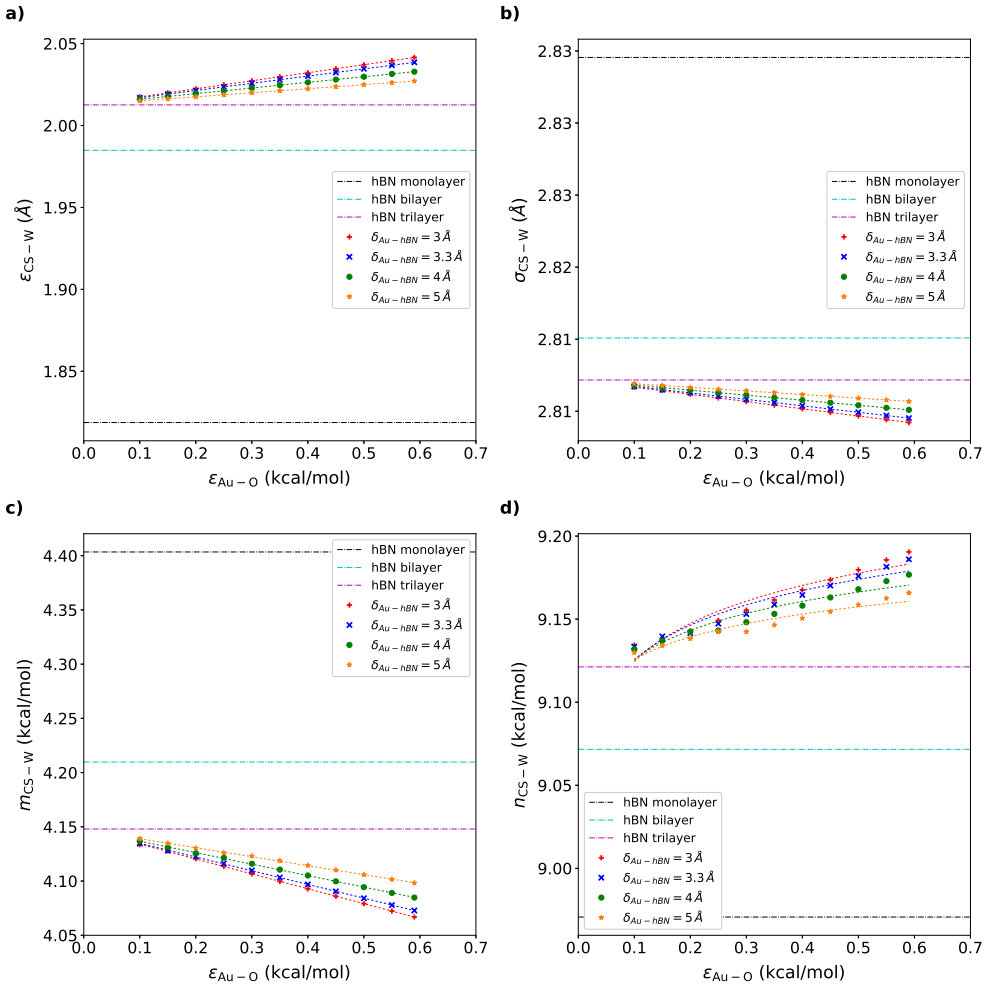

Figure S3: Parameters for the coated substrate-water interaction, obtained from the fit to a Mie potential (eq. 1 from the main article). The computed parameters correspond to a surface coated by trilayer hBN, with different contact distances ($\delta_{\mathrm{Au-hBN}}$). a) $\varepsilon_{\mathrm{CS-W}}$ b) $\sigma_{\mathrm{CS-W}}$ c) $m_{\mathrm{CS-W}}$ d) $n_{\mathrm{CS-W}}$.

Water contact angle on a substrate coated by bilayer hBN

The measured WCA for a substrate coated by hBN bilayer is presented in Figure S4. For the studied range of $\varepsilon_{\mathrm{Au-O}}$ and $\delta_{\mathrm{Au-hBN}}$, we observe that the WCA shows very little change with $\varepsilon_{\mathrm{Au-hBN}}$. This implies that the wetting translucency effect is not manifested for the multilayer hBN.

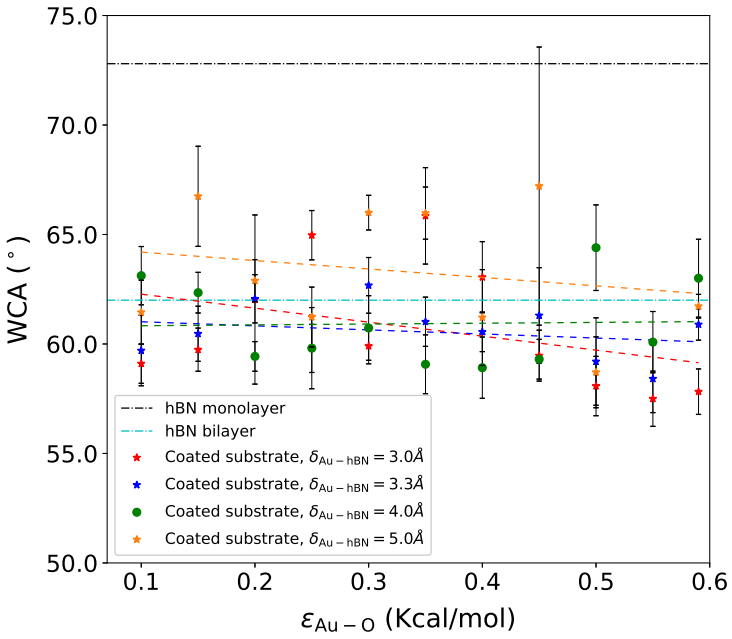

Figure S4: Water contact angle as a function of $\varepsilon_{\mathrm{Au-O}}$ for the gold-like substrate with a hBN bilayer as a coating. The dash-dotted lines in represent the water contact angle on the free standing (unsupported) hBN monolayer and bilayer.

Water contact angle on gold-supported hBN monolayer computed using the force field of Rajan et al.

Here we provide the results for the water contact angles on gold-supported hBN monolayer obtained from the MD simulations conducted by employing the recently developed force field of Rajan et al.[S1] for computing the hBN-water interactions. The parameters for this potential are summarized in Table S1. The parameters for these interactions are computed using the geometric combining rules. For a free-standing hBN monolayer, a WCA of $92.0 \pm 1.0^\circ$ is obtained. A WCA of around 82° is obtained for 2 or more free-standing hBN layers. The WCA as a function of $\varepsilon_{\mathrm{Au-O}}$ is presented in Figure S5, for a substrate coated by monolayer hBN with $\delta_{\mathrm{Au-hBN}} = 3.3$Å. We observe a behavior similar to the one reproduced by the potential of Wu et al.[S2] [see Figure 6 in the main paper]. This confirms that the wetting translucency effect of hBN monolayer is witnessed in MD simulations even with a different force field.

Table S1: Parameters for the hBN-water interactions, described by the force field of Rajan et al.[S1].

Atom type	σ (Å)	ϵ (kcal/mol)	q_i (e)
N	3.3087	0.069305	−0.907
B	3.2174	0.047343	+0.907

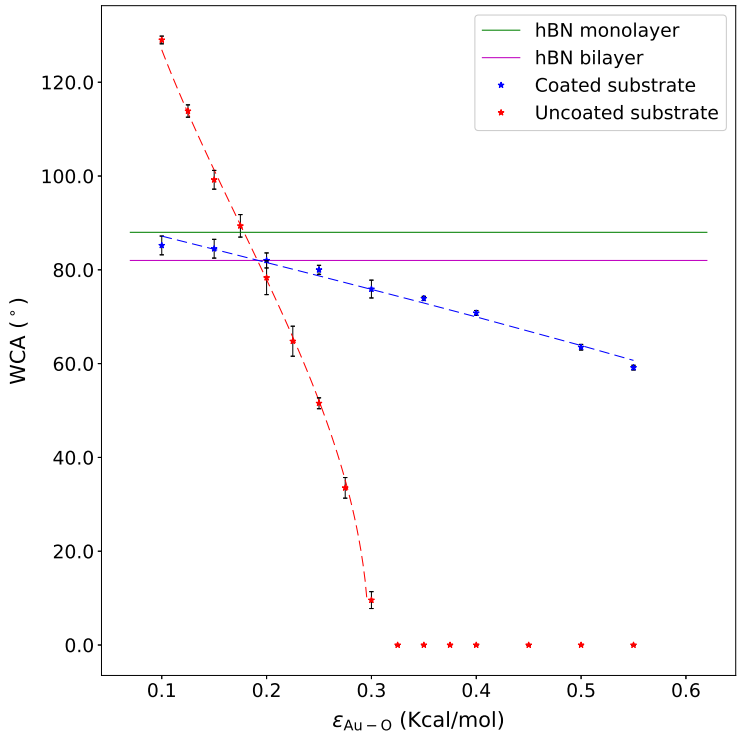

Figure S5: Water contact angle as a function of $\varepsilon_{\mathrm{AuO}}$ for the gold-like substrate without coating (red) and with an hBN monolayer as a coating (blue). The dashed lines in c) represent a linear fit between cos(WCA) and $\varepsilon_{\mathrm{AuO}}$. The solid lines represent the water contact angle on the free standing (unsupported) hBN monolayer and bilayer. The water-hBN interaction is described using the force field of Rajan et al.[S1].

References

(S1) Govind Rajan, A.; Strano, M. S.; Blankschtein, D. Ab initio molecular dynamics and lattice dynamics-based force field for modeling hexagonal boron nitride in mechanical and interfacial applications. *J. Phys. Chem. Lett.* **2018**, *9*, 1584–1591.

(S2) Wu, Y.; Wagner, L. K.; Aluru, N. R. Hexagonal boron nitride and water interaction parameters. *J. Chem. Phys.* **2016**, *144*, 164118.