

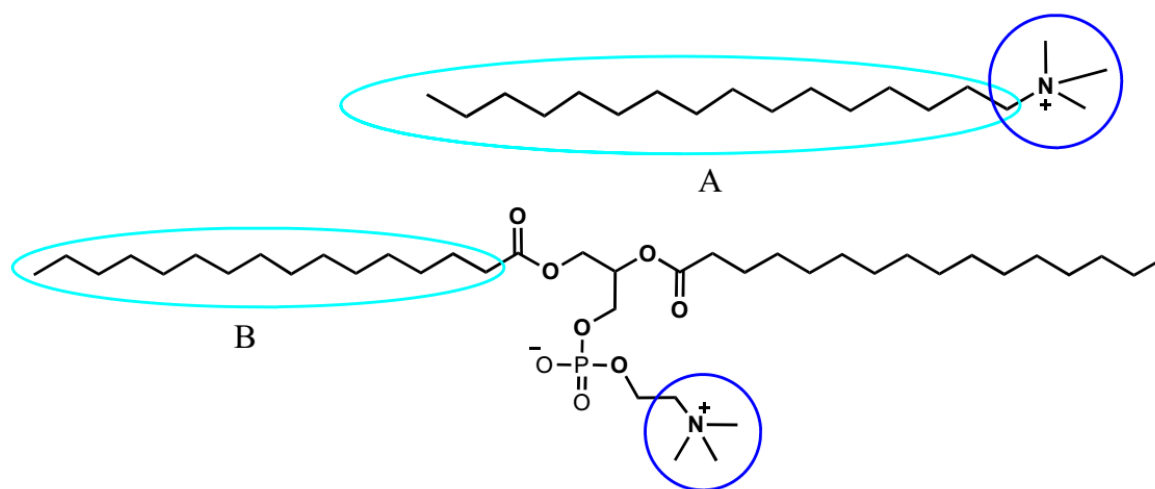
## Supplementary Information

### Molecular Dynamics Simulations of Cetyltrimethylammonium Bromide (CTAB) Micelles and their Interactions with a Gold Surface in Aqueous Solution

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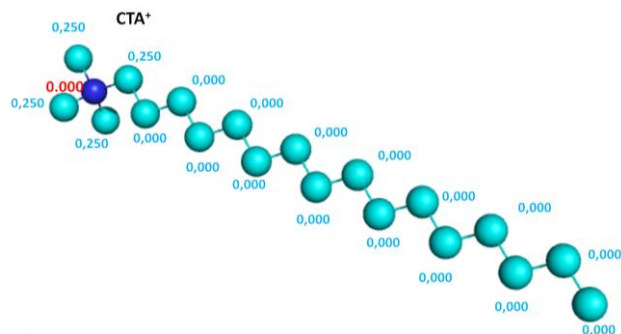
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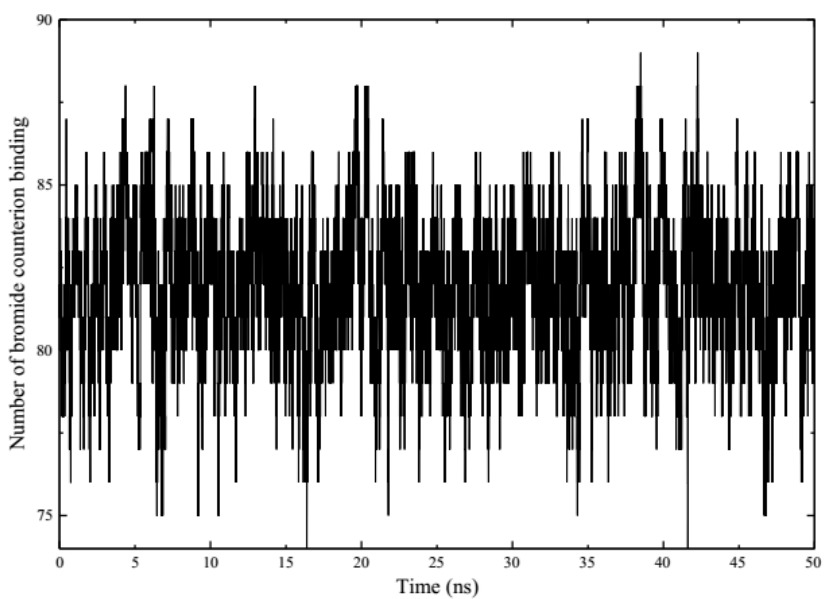
**Figure S1.** Schematic illustration showing from which fragments of DPPC lipid, the parameters of the CTA<sup>+</sup> moiety were obtained. (A) Chemical structure of the CTA<sup>+</sup> fragment; (B) chemical structure of the DPPC lipid.

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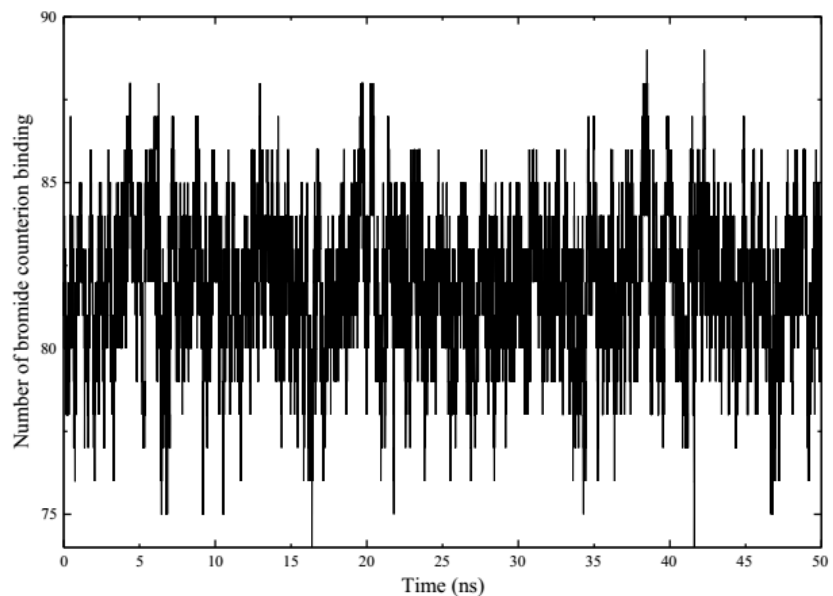


**Figure S2.** The charge distribution of the CTA<sup>+</sup> fragment.

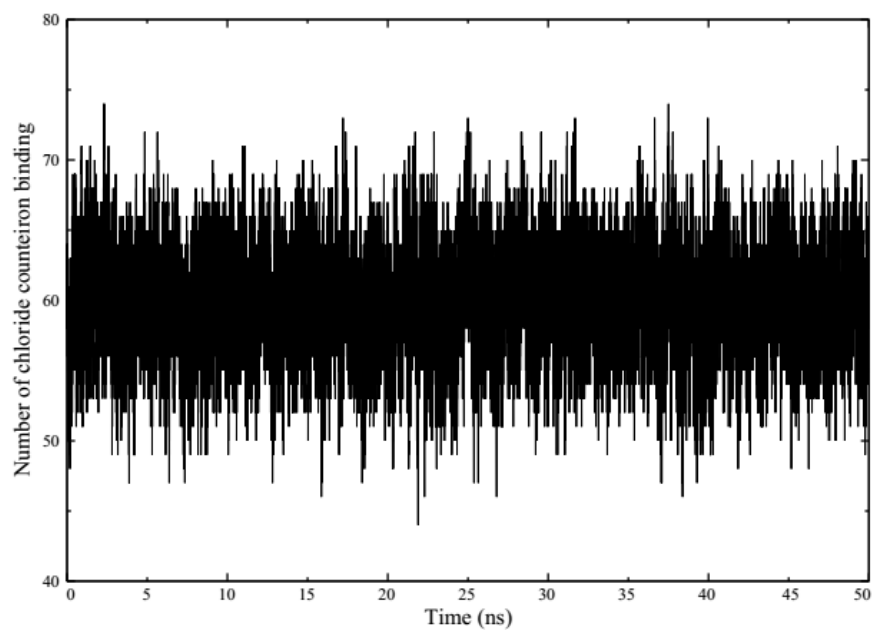
Measurements of the degree of counterion dissociation



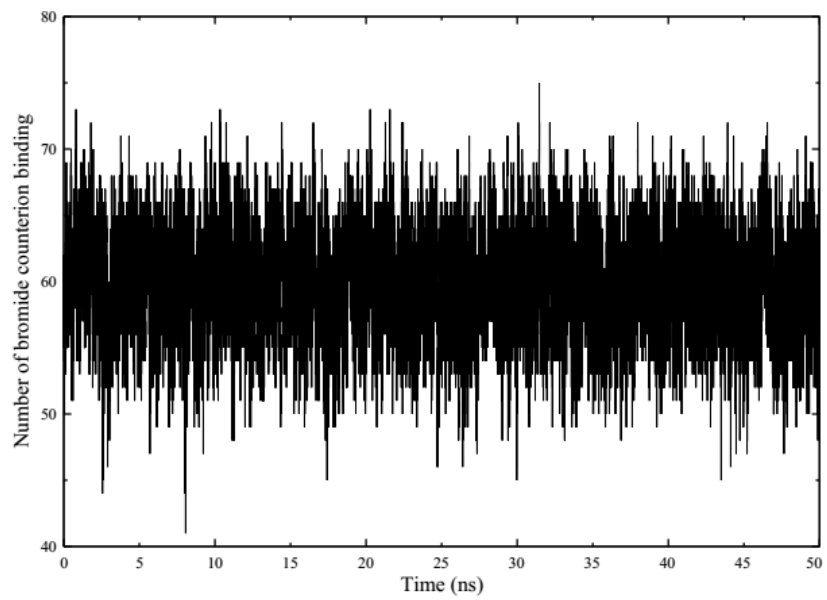
**Figure S3.** Measurements of the number of bromide counterions binding to the polar head group of the CTAB<sub>N</sub> micelle.



**Figure S4.** Measurements of the number of bromide counterions binding to the polar head group of the CTAB<sub>R</sub> micelle.



**Figure S5.** Measurements of the number of chloride counterions binding to the polar head group of the CTAC micelle.



**Figure S6.** Measurements of the number of bromide counterions binding to the polar head group of the CTAB<sub>H</sub> micelle.