Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supporting Information

Comparative Toxicity Assessment of Novel Si Quantum Dots and their Traditional Cd-based Counterparts using Bacteria Models *Shewanella oneidensis* and *Bacillus subtilis*

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S1. Growth Curve Assay: Bacterial growth rate and replication in presence of SiQDs was assessed through the bacterial growth curve assay. Bacteria were grown in minimal media to an optical density of 0.2 (cell density equivalent to approximately 2 x 10^8 colony forming units/mL) and was diluted in minimal media to achieve half the original cell concentration. The bacterial suspensions were treated with QDs at 50 mg/L, 100 mg/L, or 200 mg/L concentrations. 200 µL of treatment solutions was placed in a 96-well plate, and growth rates and bacterial concentrations were determined by measuring optical density (OD) at 600 nm using a Synergy 2 Multi-Mode Microplate Reader (BioTek, VT). No statistical significance was observed between the growth curves at different SiQD concentration when compared to the negative control.

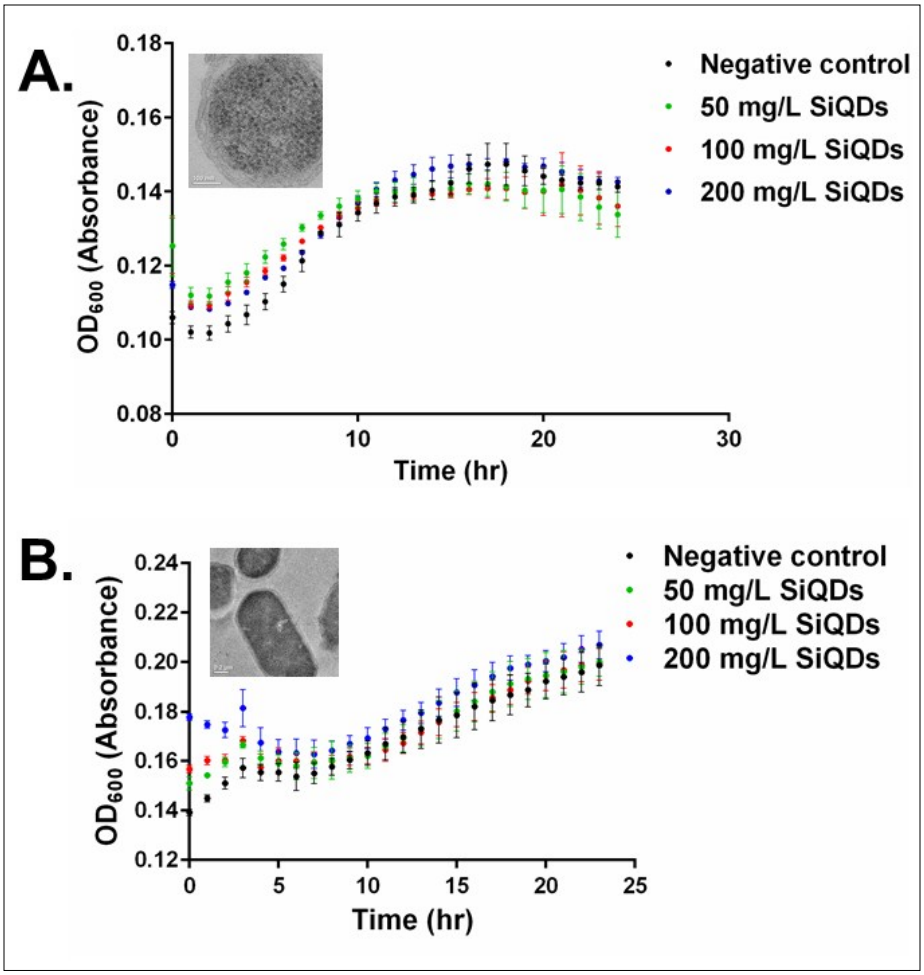

Figure S1: Growth curves of (A) S. oneidensis and (B) B. subtilis in minimal media in the presence of SiQDs.

S2. Physical characterization of Cd-based QDs: Similar to the SiQDs, DLS experiments were performed on both CdSe and CdSe/ZnS QDs to evaluate their hydrodynamic diameters both in water and HEPES buffer (the media used for biological exposures). The measurements were done at QD concentrations of 50 mg/L, 100 mg/L and 200 mg/L to monitor not only the effect of the incubating media, but also QD concentration on aggregate size. Consistent size data was obtained for CdSe QDs, as shown in Figure S2. There was no significant change in aggregate sizes in the two media, at varying QD concentrations.

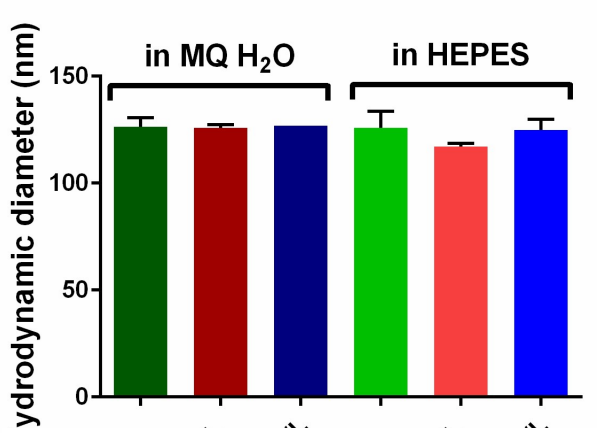

Figure S2: Dynamic light scattering data for CdSe QDs in MQ H_2O and HEPES buffer. No significant difference in hydrodynamic diameter is observed for the two media or among different nanoparticle concentrations.

The DLS data for the CdSe/ZnS QDs fluctuated between replicates, possibly due to interference posed by the fluorescence of the QDs and, thus, is not reported here. The zeta potential of the CdSe QDs were measured to be - 66.37 ± 9.2 mV, and that of CdSe/ZnS was measured to be - 90.6 ± 0.5 mV.

S3. Cryogenic TEM of SiQDs on Hydrophilic and Hydrophobic Grids: Cryogenic TEM was performed to accurately size SiQDs and assess agglomeration. To prepare the samples for analysis, the SiQDs were suspended in ultrapure water at a concentration of 3 mg mL^{-1}. The SiQDs were plunge frozen on hydrophobic lacey carbon crids for cryogenic TEM. Images reveal that agglomerates were present, and the ice poorly spread on the grids (Figure S3 A-C). In effort to improve sample preparation, the lacey carbon grids were made hydrophilic through plasma glow discharge. Imaging of samples on these grids revealed more uniform thin vitrified ice,

monodisperse SiQDs, and formations of agglomerates (Figure S3 D-F). Of note, there was also presence of larger, dark contrast objects on the grids, likely due to ethane contamination or ice crystals (Figure S3 F, yellow box). All images were analyzed with the free NIH ImageJ software. Measurements were made by drawing a line segment across the scale bar and setting the pixel/nm scale. The diameter of the particles was measured by using the oval draw tool to fit an ellipse diameter. A minimum of 300 nanoparticle diameters was measured for each preparation.

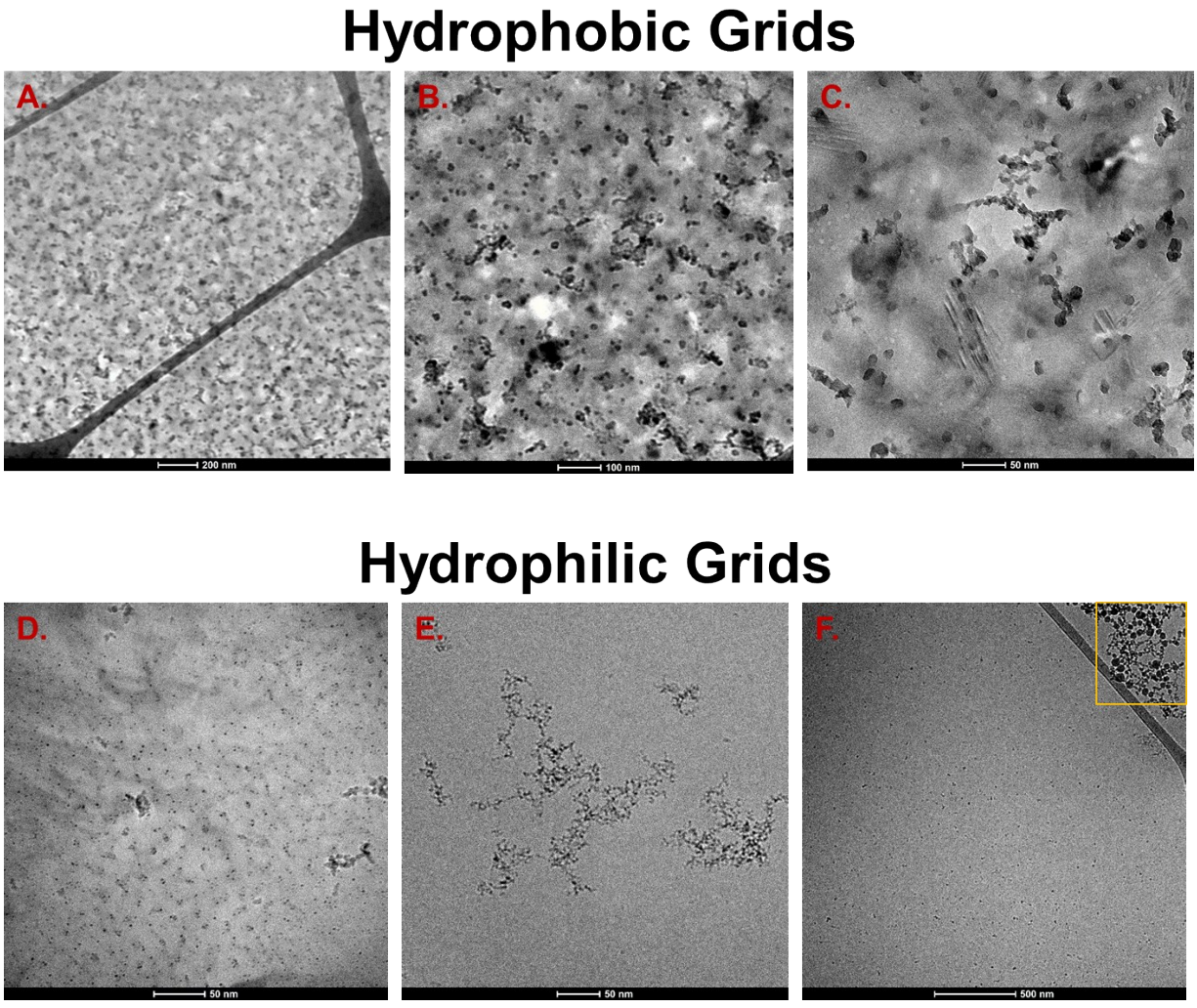

Figure S3: Cryogenic transmission electron micrographs of SiQDs on hydrophobic (top) and hydrophilic grids (bottom). Samples were prepared with a concentration of 3 mg mL^{-1}. A. Dispersion of large particles on the hydrophobic grid. B. Poor ice spreading and possible contamination surrounding SiQDs. C. Representative thick ice and crystalline ice. D.

Monodisperse SiQDs with average diameter of 3.8 ± 0.04 nm (n=400, mean ± std. error). E. Formation of aggregate particles in vitrified ice. F. Dispersion of larger particles or agglomerates with average diameter of 19.2 ± 0.2 nm (n=300, mean ± std. error). Probable ice or ethane contamination indicated by yellow box.