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Electronic Supplementary Information for:

Adsorption of III/V ions (In(III), Ga(III) and As(V)) to SiO_2, CeO_2 and Al_2O_3 nanoparticles used in the semiconductor industry

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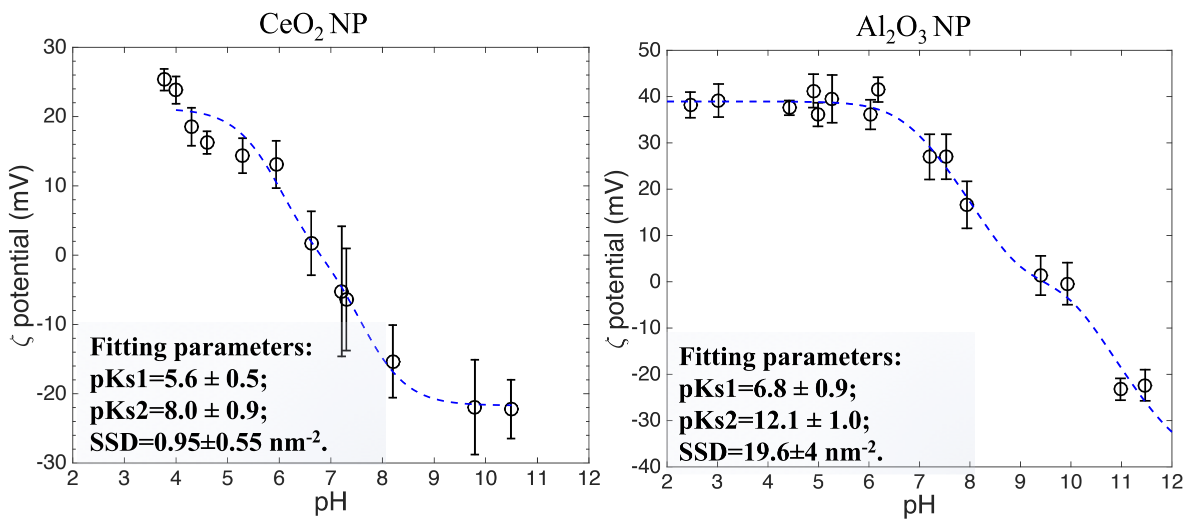

Figure S1. Zeta-potential of CeO_2 and Al_2O_3 NPs as a function of pH. The markers are the experimental measurement, and the solid line is the diffusive layer model fit (Table 1). The model fit parameterizes the pK_s values of surface –OH groups and the surface site density (SSD), which are given with the charts.

Table S1. Hydrolysis of In(III), Ga(III) and As(V) ions and the equilibrium constants.

Equation	Equilibrium Constant (logK)	Value	Source
$HAsO_4^{2-} \rightleftarrows H^+ + AsO_4^{3-}$	$\log(K_1^{As})$	-11.6	Drever, 1997[3]
$H_2AsO_4^{-} \rightleftarrows 2H^+ + AsO_4^{3-}$	$\log(K_2^{As})$	-18.36	Drever, 1997[3]
$H_3AsO_4 \rightleftarrows 3H^+ + AsO_4^{3-}$	$\log(K_3^{As})$	-20.6	Drever, 1997[3]
$In^{3+} + H_2O \rightleftarrows In(OH)^{2+} + H^+$	$\log(K_1^{In})$	-3.48	Biryuk et al., 1986[4]
$In^{3+} + 2H_2O \rightleftarrows In(OH)_2^{+} + 2H^+$	$\log(K_2^{In})$	-7.67	Biryuk et al., 1986[4]
$In^{3+} + 3H_2O \rightleftarrows In(OH)_3^{+} + 3H^+$	$\log(K_3^{In})$	-12.75	Biryuk et al., 1986[4]
$Ga^{3+} + H_2O \rightleftarrows Ga(OH)^{2+} + H^+$	$\log(K_1^{Ga})$	-2.87	Biryuk and Nazarenko, 1973[5]
$Ga^{3+} + 2H_2O \rightleftarrows Ga(OH)_2^{+} + 2H^+$	$\log(K_2^{Ga})$	-6.55	Biryuk and Nazarenko, 1973[5]
$Ga^{3+} + 3H_2O \rightleftarrows Ga(OH)_3^{+} + 3H^+$	$\log(K_3^{Ga})$	-11.07	Biryuk and Nazarenko, 1973[5]
$Ga^{3+} + 4H_2O \rightleftarrows Ga(OH)_4^{-} + 4H^+$	$\log(K_4^{Ga})$	-17.3	Vagramjan and Leshawa, 1967[6]

Relate the surface site density (SSD) to the NP size for colloidal SiO_2 NPs

For a spherical colloidal SiO_2 NP, we denote p as the number of Si atoms across the diameter of the sphere, in the unit of nm^{-1}. The total number of Si atoms in this sphere is:

$$N_t = \frac{\pi \bullet p^3}{6} \quad \text{Eq(S1)}$$

where, N_t is the total number of Si in the sphere.

The weight of this SiO_2 NP is calculated as:

$$w_{NP} = \frac{N_t \bullet MW}{N_A} = \frac{\pi \bullet p^3 \bullet MW}{6N_A} \quad \text{Eq(S2)}$$

where, w_{NP} is the weight of the SiO_2 NP and MW is the molecular weight of SiO_2 (28.1 $g \bullet mol^{-1}$).

w_{NP} is also calculated as:

$$w_{NP} = \rho \bullet \frac{1}{6} \bullet \pi \bullet d^3 \quad \text{Eq(S3)}$$

where ρ is the density of colloidal SiO_2 NPs and d is the particle diameter.

Eq(S2) and Eq(S3) give:

$$p = \left(\frac{\rho \bullet N_A}{MW} \right)^{\frac{1}{3}} \bullet d \quad \text{Eq(S4)}$$

For colloidal SiO_2 NPs, ρ is 2.2 $g \bullet cm^{-3}$ and MW is 28.1 $g \bullet mol^{-1}$. Substituting these values into Eq(S4) gives:

$$p = 2.80d \quad \text{Eq(S5)}$$

where d is in nm.

Based on Eq(S1), the number of Si atom on the sphere surface (N_s) is calculated as:

$$N_s = \frac{1}{6}\pi\left(p^3 - (p-2)^3\right) \quad \text{Eq(S6)}$$

Given the assumption that each Si atom on the surface carries one –OH group, SSD is calculated as:

$$SSD = \frac{N_s}{\pi \bullet d^2} \quad \text{Eq(S7).}$$

Substituting Eq(S5) and Eq(S6) into Eq(S7) gives:

$$SSD = 7.86 + \frac{1.33}{d^2} - \frac{5.61}{d} \quad \text{Eq(S8)}$$

where d is in nm.

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