Supplementary Data for

Acellular oxidative potential assay for screening of amorphous silica nanoparticles

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Running Title: Oxidative potential of amorphous nano silica particles

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Functional Group Surface Coverage Calculation:

Surface area of SiNPs was based on their TEM size-based average diameter. The SiNPs were assumed as spherical in shape. An example for C11-COOH-modified SiNP-15 nm is presented below;

Surface Area for 17.2 nm particles

The surface area of 17.2 nm particles = $4 * 3.14 * (8.6 * 10^{-9})^2$ $m^2 = 9.3 * 10^{-16}$ m^2

Volume of a 17.2 nm particle = $4/3 * 3.14 * (8.6 * 10^{-7}$ cm$)^3 = 2.7 * 10^{-18}$ c.c

Mass of a 17.2 nm SiO_2 nanoparticle = $2.7 * 10^{-18}$ c.c $* 2.2$ g/c.c $= 5.94 * 10^{-18}$ g.

# of particles in 1 g of particles = $1/5.94 * 10^{-18} = 1.7 * 10^{17}$

The surface area of 1 g of 17.2 nm particles = $(1.68 * 10^{17} * 9.3 * 10^{-16})$ $m^2 = 156.6$ m^2

Surface Density for 17.2 nm particles

From Figure S8a, % weight loss of ligand from 17.2 nm = 8.32 %, (i.e. 83.2 mg of ligands/ 1 g of SiNP surface.

% weight loss of ligands per m^2 of particles = weight of ligands/surface area per 1 g of SiNPs = 83.2 mg / 156.6 m^2 = 0.53 mg/m^2

Molecular weight of surface ligand (11-cyanoundecyltrisiloxy group) = 256.5

μmol in 0.64 mg of ligands = $0.53 * 1000/256.5 = 2.07$

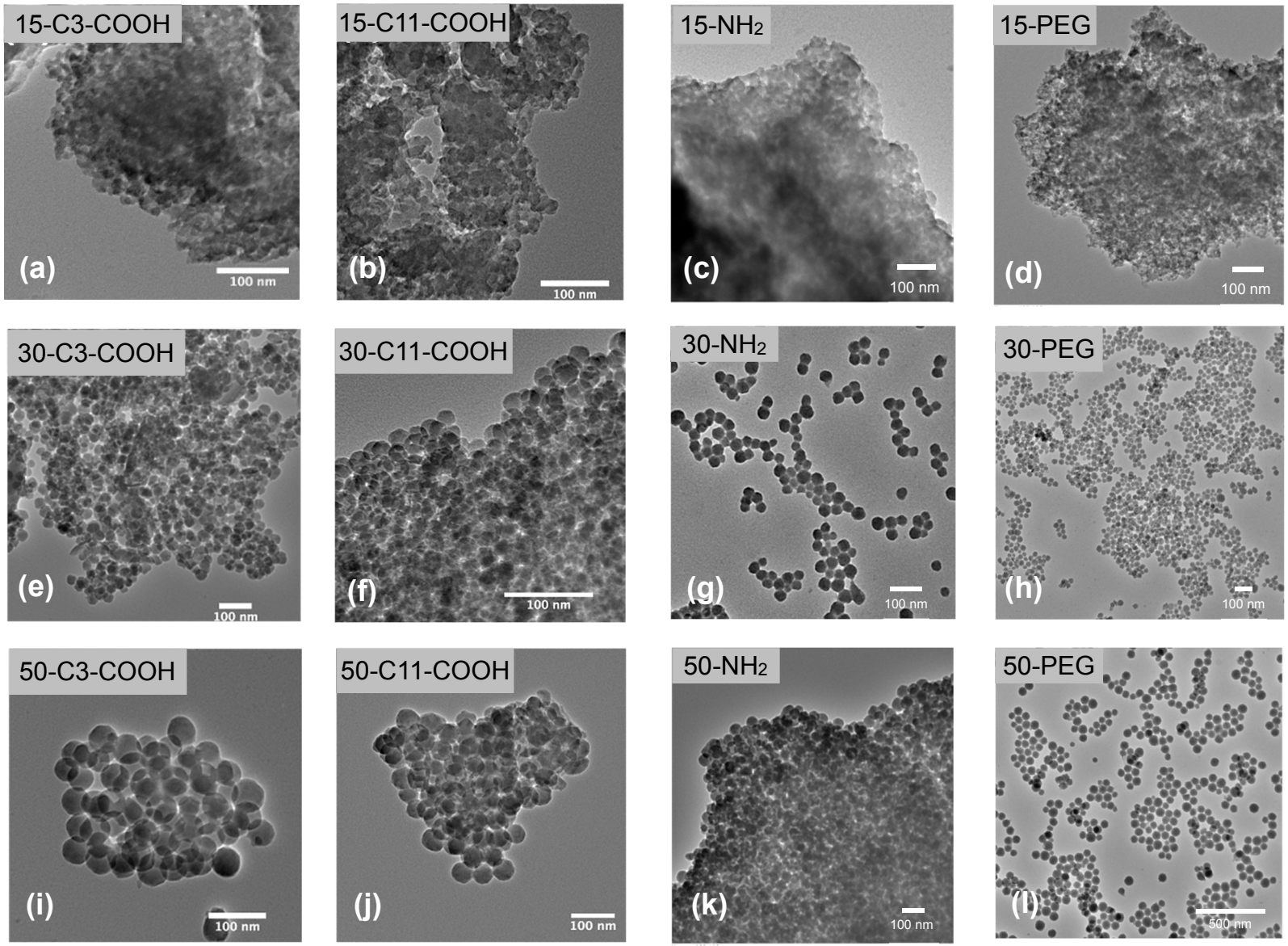
Similar calculation was performed for all other surface-modified SiNPs, with the the following molecular weights applied as required;

3-cyanoundecyltrisiloxy group (C3-COOH modification) molecular weight = 146.4

3-aminopropyltrisiloxy group (NH_2 modification) molecular weight = 133.3

2-[methoxy(polyethyleneoxy)-propyl]trisiloxy group (PEG modification) molecular weight = 610

Figure S1: TEM Analysis Results for Surface-Modified SiNPs; (a-d) 15 nm, (e-h) 30 nm, (i-l) 50 nm, (m-p) 75 nm, (q-t) 100 nm C3-COOH, C11-COOH-NH_2 and PEG-modified SiNP's



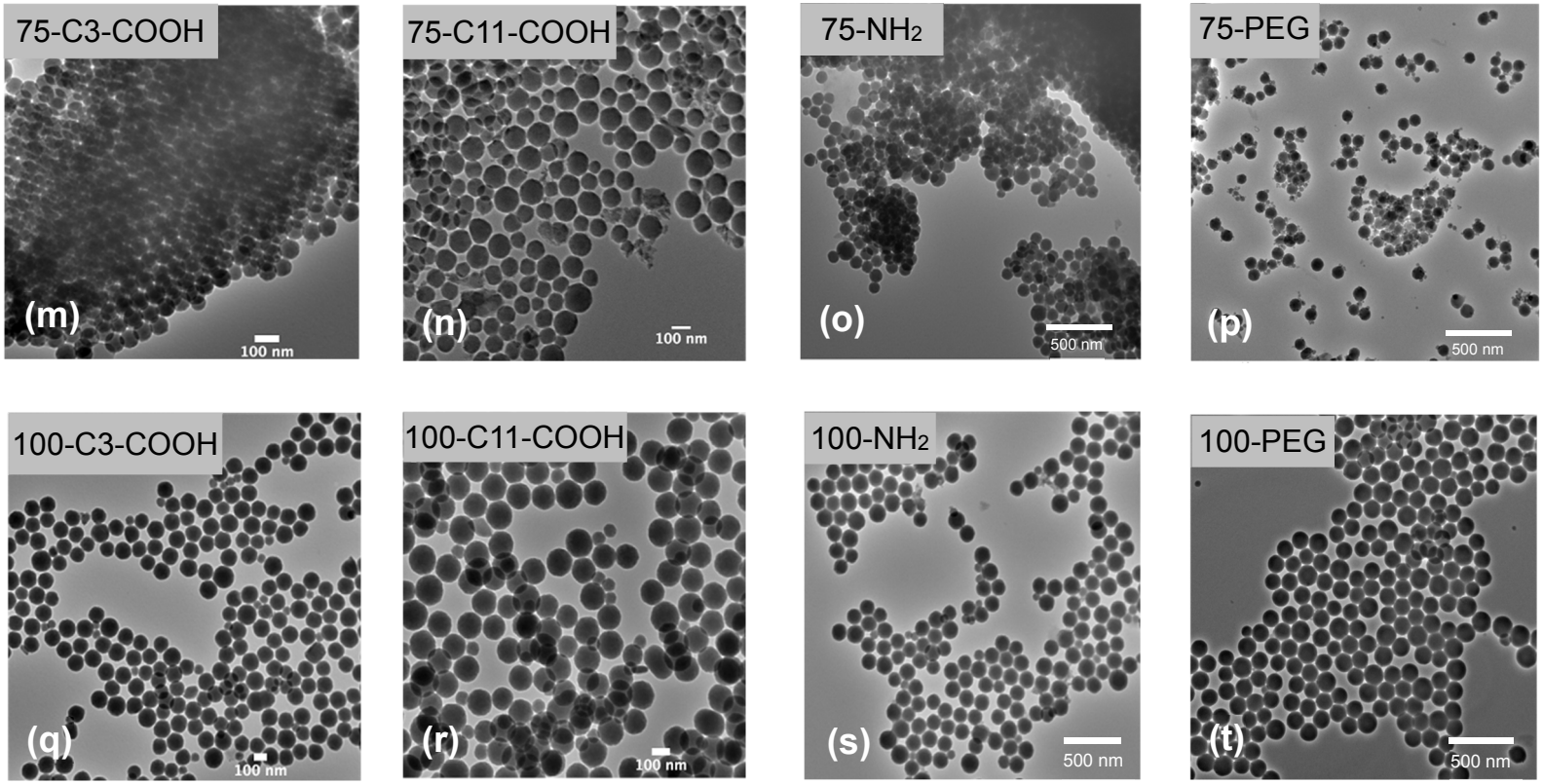

75-C3-COOH
(m)
100 nm
75-C11-COOH
(n)
100 nm
75-NH2
(o)
500 nm
75-PEG
(p)
500 nm
100-C3-COOH
(q)
100 nm
100-C11-COOH
(r)
100 nm
100-NH2
(s)
500 nm
100-PEG
(t)
500 nm

Figure S2: Powder XRD patterns of SiNPs with of various sizes (15, 30, 50, 75 and 100 nm)

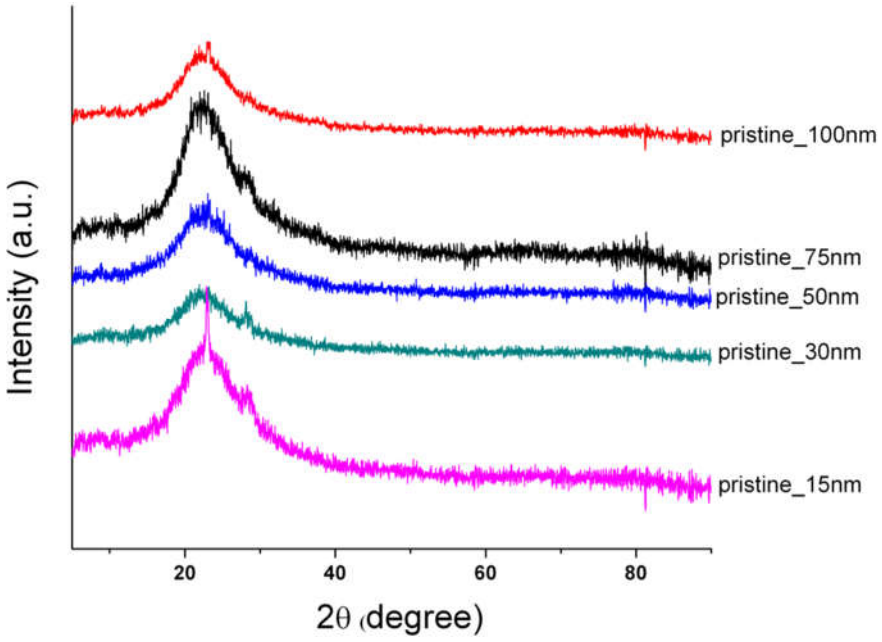


Figure S3: Intrinsic oxidative capacity of SiNPs and reference particles based on DTT depletion at different time points. The increased DTT substrate depletion is indicated by higher negative values of the DTT absorbance relative to the spontaneous depletion of DTT in the blank sample (subtracted from the absorbance values of the samples). Note: 3 min was the minimum time taken for the processing of the samples prior to oxidative potential measurement

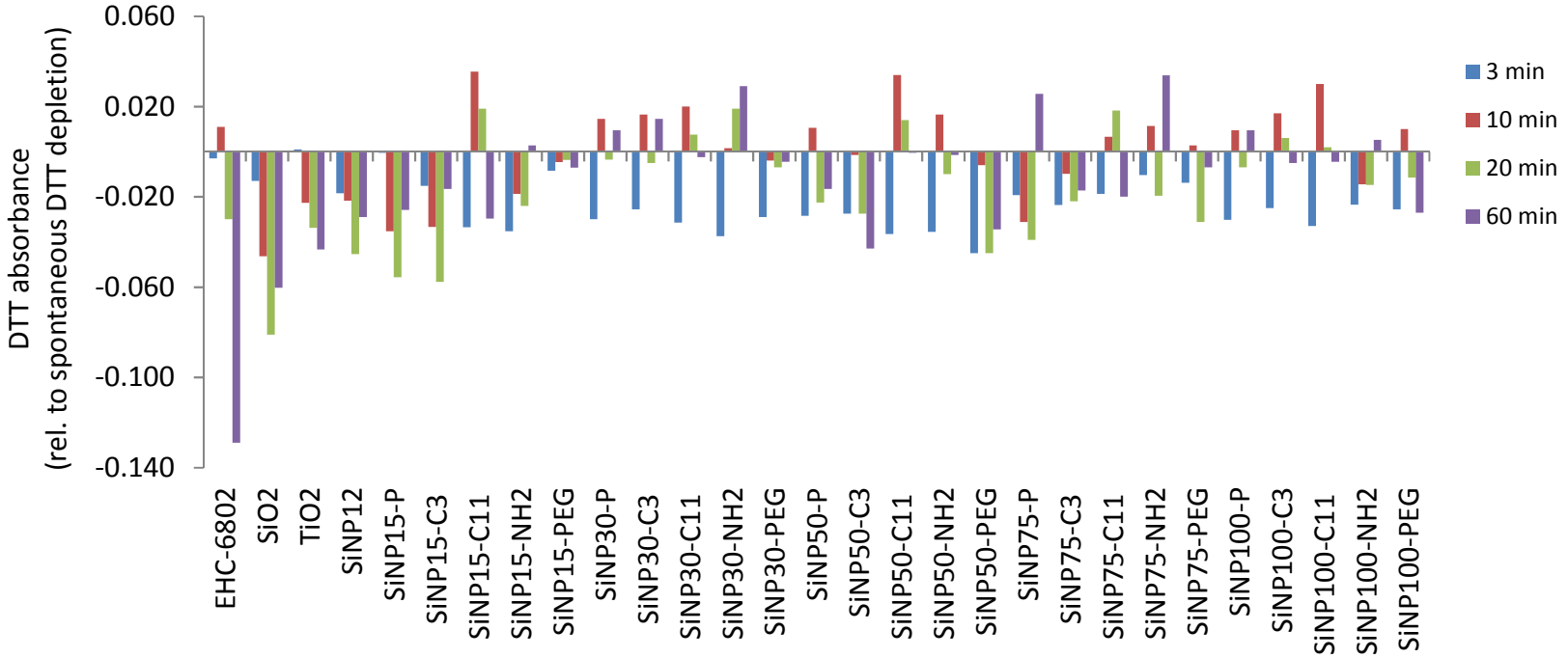


Table S1: Elemental composition of the pristine SiNPs as quantified by ICP-MS

Elements (ppm)	SiNP15-P	SiNP30-P	SiNP50-P	SiNP75-P	SiNP100-P
$_{7}$Li [No He]	0.35	0.111	0.09	0.12	0.14
$_{9}$Be [No He]	0.03	0.01	0.02	0.00	0.00
$_{11}$B [No He]	14.03	11.48	10.61	8.71	4.95
$_{24}$Mg [No He]	12.10	20.18	18.54	18.43	18.12
$_{27}$Al [No He]	607.22	396.63	625.98	308.81	269.24
$_{43}$Ca [No He]	23.83	25.82	28.21	19.24	13.71
$_{45}$Sc [He_2]	0.36	0.10	0.12	0.06	0.04
$_{47}$Ti [No He]	133.57	102.26	141.46	66.61	46.84
$_{51}$V [He_2]	0.59	0.06	0.52	0.07	0.07
$_{52}$Cr [No He]	4.88	3.88	14.27	10.14	9.82
$_{59}$Co [He_2]	0.08	0.05	0.13	0.11	0.10
$_{60}$Ni [He_2]	1.94	1.36	5.57	4.22	4.23
$_{63}$Cu [No He]	1.56	0.56	2.48	1.22	0.97
$_{66}$Zn [No He]	4.37	3.08	3.92	2.99	7.31
$_{71}$Ga [No He]	0.16	0.07	0.15	0.06	0.04
$_{72}$Ge [He_2]	0.36	0.28	0.59	0.44	0.44
$_{75}$As [No He]	0.14	0.13	0.22	0.17	0.22
$_{77}$Se [No He]	0.10	0.15	0.47	0.12	0.11
$_{85}$Rb [No He]	0.11	0.02	0.04	0.01	0.01
$_{88}$Sr [No He]	2.65	2.09	3.48	1.26	0.38
$_{89}$Y [He_2]	0.58	0.67	0.45	0.48	0.31
$_{90}$Zr [No He]	25.48	27.64	30.05	22.12	18.95
$_{93}$Nb [He_2]	0.37	0.40	0.43	0.25	0.16
$_{95}$Mo [No He]	0.09	0.05	0.16	0.10	0.10
$_{107}$Ag [He_2]	0.49	0.54	0.67	0.44	0.46
$_{111}$Cd [No He]	0.04	0.05	0.05	0.42	0.04
$_{118}$Sn [No He]	0.43	0.42	0.42	0.36	0.36
$_{121}$Sb [No He]	0.06	0.06	0.09	0.13	0.10
$_{137}$Ba [No He]	3.02	7.16	6.80	4.36	0.81
$_{139}$La [He_2]	0.88	1.51	0.76	1.03	0.75
$_{140}$Ce [He_2]	2.54	2.51	2.48	1.28	0.43
$_{141}$Pr [He_2]	0.20	0.31	0.16	0.22	0.17
$_{146}$Nd [He_2]	0.72	1.11	0.59	0.79	0.62
$_{147}$Sm [He_2]	0.14	0.19	0.11	0.14	0.12
$_{157}$Gd [He_2]	0.12	0.18	0.10	0.14	0.11
$_{163}$Dy [He_2]	0.14	0.18	0.11	0.13	0.11
$_{166}$Er [He_2]	0.10	0.10	0.08	0.06	0.04
$_{178}$Hf [He_2]	0.70	0.75	0.78	0.59	0.50
$_{181}$Ta [He_2]	0.17	0.05	0.05	0.03	0.02
$_{182}$W [He_2]	1.93	2.41	0.54	0.12	0.17
$_{201}$Hg [He_2]	0.01	0.01	0.02	0.01	0.02
$_{208}$Pb [No He]	0.48	0.20	0.20	0.22	0.13
$_{232}$Th [He_2]	0.52	0.46	0.42	0.28	0.20