Supplementary Information (SI) for Environmental Science: Nano.

Are Ni-SiC Nanoparticle Electroplated Coatings a Safer Alternative to Hard Chromium? A Comprehensive Aging, Toxicity, and *In Silico* Studies to Assess Safety by Design

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Supplementary Information:

Table S1- Composition of aging media used in the studies

Simulated Media	Chemical Composition	References
Artificial Sea Water (ASW) (pH- 7.5) (1L)	NaCl (24.60 g); $NaHCO_3$ (0.180 g); KCl (0.670 g); $CaCl_2$ (1.360 g); $MgSO_4.7H_2O$ (6.290 g)	12
Waste Water (WW) (pH- 7.1) (1L)	Milk powder (150 mg); Starch (80 mg); Na-acetate (103 mg); Yeast (24 mg); NH_4Cl (21.7 mg); Urea (12.8 mg); KH_2PO_4 (13.2 mg); $NaHCO_3$ (600 mg)	13
1mM $NaNO_3$ (pH 6.5- 7) (1L)	$NaNO_3$ (0.085 g)	12
Synthetic Sweat (SS) (1L)	H_2O (18.01 g/mol), NaOH (39.99 g/mol), NaCl (58.44 g/mol),NH_4Cl (53.49 g/mol), $CH_3CHOHCOOH$ (0.07 g/mol), NH_2CONH_2 (0.05 g/mol), H_3COOH (60.05 g/mol)	14

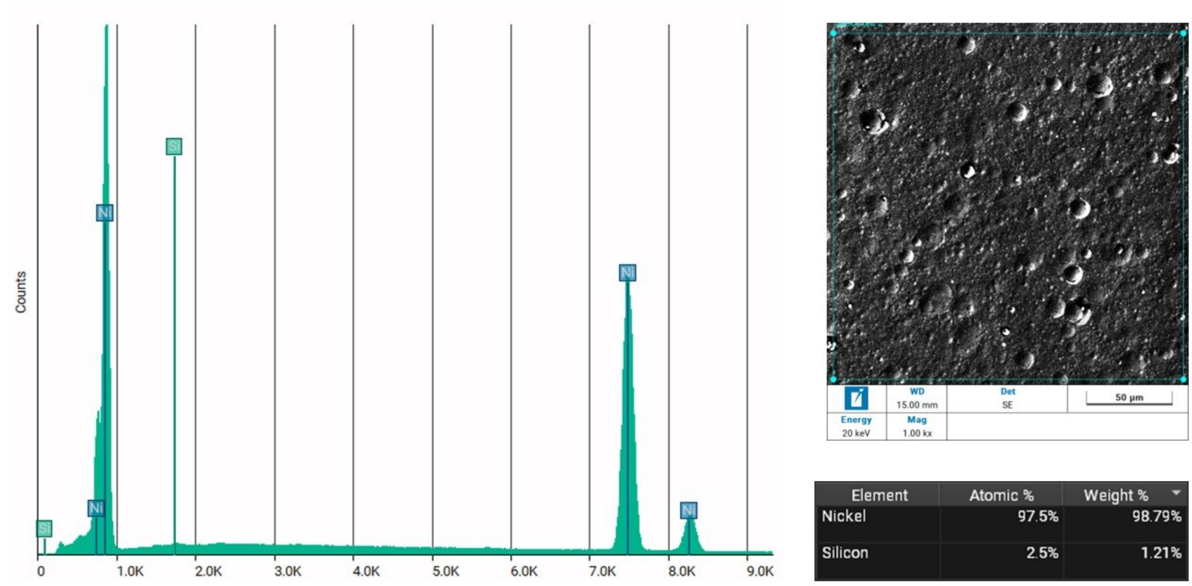

Figure S1. *EDS analysis of* Ni-SiC nanocomposite *coatings.*

Table S2: *Release of Ni and SiC from Ni watt type and* Ni-SiC nanocomposite *electroplated coatings on exposure to cell culture media (n=3)*

Sample	**Ni (µg/mL)**		**Si (µg/mL)**	
Ni watt type	24 h	29.98±1.25	No Si release	
	48 h	40.41±6.8		
	72 h	60.91±4.6		
Ni watt/SiC NPs	24 h	61.4±2.5	24 h	101.2±5.1
	48 h	87.6±5.1	48 h	230.9±6.9
	72 h	143.1±15.1	72 h	320.96±4.2

Modelling Section-

Golbraikh and Tropsha criteria

According to Golbraikh and Tropsha[1–3] a regression model is considered predictive if all of the conditions presented in Table S2 are satisfied.

$$r^2 = \left(\frac{\sum_{i=1}^{N} (y_i - \bar{y})(\hat{y}_i - \bar{\hat{y}}_i)}{\sqrt{\sum_{i=1}^{N} (y_i - \bar{y})^2 \sum_{i=1}^{N} (\hat{y}_i - \bar{\hat{y}}_i)^2}} \right)^2 \quad \text{[Eq. SI1]}$$

$$R_0^2 = 1 - \frac{\sum_{i=1}^{N}\left(\hat{y}_i - \hat{y}_i^{r_0}\right)^2}{\sum_{i=1}^{N}\left(\hat{y}_i - \bar{\hat{y}}_i\right)^2}, where\ \hat{y}_i^{r_0} = k'y$$ [Eq. SI2]

$$R_0^{'2} = 1 - \frac{\sum_{i=1}^{N}\left(y_i - y_i^{r_0}\right)^2}{\sum_{i=1}^{N}\left(y_i - \bar{y}\right)^2}, where\ y_i^{r_0} = k\hat{y}$$ [Eq.SI3]

$$k = \frac{\sum_{i=1}^{N} y_i \hat{y}_i}{\sum_{i=1}^{N} \hat{y}_i^2}$$ [Eq. SI4]

$$k' = \frac{\sum_{i=1}^{N} y_i \hat{y}_i}{\sum_{i=1}^{N} y_i^2}$$ [Eq. SI5]

Where N, is the number of samples, y_i and $\hat{y}_i$, are the actual and predicted endpoint values of the i^{th} sample respectively, and $\bar{y}$ and $\bar{\hat{y}}_i$, are the average endpoint values of the experimental and predicted values respectively.

Table S3: Model acceptability criteria as defined by Golbraikh and Tropsha[1–3].

Statistic	Rule
r^2	> 0.6
Q_{ext}^2	> 0.5
$\frac{r^2 - R_0^2}{r^2}\ or\ \frac{r^2 - R_0^{'2}}{r^2}$	< 0.1
$k\ or\ k'$	$\in [0.85, 1.15]$
$\left\lvert R_0^2 - R_0^{'2} \right\rvert$	< 0.3

References

1. Golbraikh, A. & Tropsha, A. Beware of q^2! *J. Mol. Graph. Model.* **20**, 269–276 (2002).

2. Tropsha, A., Gramatica, P. & Gombar, V. K. The Importance of Being Earnest: Validation is the Absolute Essential for Successful Application and Interpretation of QSPR Models. *QSAR Comb. Sci.* **22**, 69–77 (2003).

3. Melagraki, G. & Afantitis, A. Enalos KNIME nodes: Exploring corrosion inhibition of steel in acidic medium. *Chemom. Intell. Lab. Syst.* **123**, 9–14 (2013).

Release data used for modelling

Sample	Sample	F	DC	I dens	Area	I real	M1	M2	dm	Time	Theor m	Eff	Thickne	Pristine/	Number	Coating	Concent	Concent	Concent	Concent	Ionic Ni	TEM	Surface	Morphol	Exposin	Media	Zeta	Time of	Temper	Chemic	Ni ion
MS1-	1	10	50	1	70	0.7	17.4212	18.1545	0.7333	120	0.77	96	12.2	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	1mM	7.1	-10.80	7	37 °C	Nirates	4.08
MS3-	2	10	50	1	102	1.1	16.1352	16.6187	0.4835	120	1.2	40	5.5	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	1mM	7.1	-10.80	7	37 °C	Nirates	6.48
MS4-	3	10	50	2	102	2	16.4173	17.3072	0.8899	120	2.19	41	10.1	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	1mM	7.1	-10.80	7	37 °C	Nirates	4.8
MS7-	4	10	50	2	102	2	19.4487	23.572	4.1233	240	4.38	94	47	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	1mM	7.1	-10.80	7	37 °C	Nirates	3.65
MS8-	5	10	50	2	102	2	19.4828	23.524	4.0412	240	4.38	92	46.1	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	1mM	7.1	-10.80	7	37 °C	Nirates	3.99
MS9-	6	10	50	2	102	2.04	19.335	24.4728	5.1378	300	5.58	92	58.6	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	1mM	7.1	-10.80	7	37 °C	Nirates	3.44

MS10-SARYD	7	10	50	2	108	2.16	19.5306	25.0028	5.4722	300	5.91	93	58.9	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica-	1mM NaNO3	7.1	-10.80	7	37 °C	Nirates of Ni	4.48
MS_Old_2	8	10	50	2	70	1.4	15.0442	17.239	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica-	1mM NaNO3	7.1	-10.80	7	37 °C	Nirates of Ni	2.08
MS_Old_10	9	10	50	2	70	1.4	15.0412	17.236	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica-	1mM NaNO3	7.1	-10.80	7	37 °C	Nirates of Ni	9.15
MS_MS_11	10	10	50	2	108	2.16	19.3387	24.8853	5.5466	300	5.91	93	58.9	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica-	1mM NaNO3	7.1	-10.80	7	37 °C	Nirates of Ni	4.13
MS12-SARYD	11	10	50	2	108	2.16	19.2772	24.791	5.5138	300	5.91	94	59.7	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica-	1mM NaNO3	7.1	-10.80	7	37 °C	Nirates of Ni	7.56
MS 15-SARYD	12	10	50	2	108	2.16	19.1637	24.7323	5.5686	300	5.91	93	59.4	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica-	1mM NaNO3	7.1	-10.80	7	37 °C	Nirates of Ni	7.06
MS_Old_2	13	10	50	2	70	1.4	15.0472	17.242	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica-	1mM NaNO3	7.1	-10.80	7	37 °C	Nirates of Ni	6.52

MS_Old_7	14	10	50	2	70	1.4	15.0412	17.236	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica	1mM NaNO3	7.1	-10.80	7	37 °C	Nirates of Ni	3
MS_Old_8	15	10	50	2	70	1.4	15.0412	17.236	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica	1mM NaNO3	7.1	-10.80	7	37 °C	Nirates of Ni	4.94
MS_Old_9	16	10	50	2	70	1.4	15.0397	17.2345	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica	1mM NaNO3	7.1	-10.80	7	37 °C	Nirates of Ni	6
Ni2	17		##	2	70	1.4	35.364	39.162	3.798	150	3.83	99	63.1	Aged	3	Ni coating	0	NA	300	35	NA	0	NA	NA	1mM NaNO3	7.1	-10.80	7	37 °C	Nitrate of Ni	6.780077
Ni5	18	10	50	2	70	1.4	34.639	37.99	3.351	290	3.45	97	55.7	Aged	3	Ni coating on Brass	0	NA	300	35	NA	0	NA	NA	1mM NaNO3	7.1	-10.80	7	37 °C	Nitrate of Ni	3.361200585
Ni6	19	10	50	2	70	1.4	35.1	38.85	3.75	300	3.83	98	62.3	Aged	3	Ni coating	0	NA	300	35	NA	0	NA	NA	1mM NaNO3	7.1	-10.80	7	37 °C	Nitrate of Ni	6.449059
SABY new	20	10	50	2	100	2	98.35	103.44	5.09	300	5.47	93	59.2	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica	1mM NaNO3	7.1	-10.80	7	37 °C	Nitrate of Ni	5.83782

MS1-SARYD	1	10	50	1	70	0.7	17.4212	18.1545	0.7333	120	0.77	96	12.2	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherical	Simulated Sweat	5.5	-9.60	7	37 °C	Cl, OH, NO3	781.5872
MS3-SARYD	2	10	50	1	102	1.1	16.1352	16.6187	0.4835	120	1.2	40	5.5	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherical	Simulated Sweat	5.5	-9.60	7	37 °C	Cl, OH, NO3	716.4566
MS4-SARYD	3	10	50	2	102	2	16.4173	17.3072	0.8899	120	2.19	41	10.1	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherical	Simulated Sweat	5.5	-9.60	7	37 °C	Cl, OH, NO3	851.7789
MS7-SARYD	4	10	50	2	102	2	19.4487	23.572	4.1233	240	4.38	94	47	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherical	Simulated Sweat	5.5	-9.60	7	37 °C	Cl, OH, NO3	649.0973
MS8-SARYD	5	10	50	2	102	2	19.4828	23.524	4.0412	240	4.38	92	46.1	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherical	Simulated Sweat	5.5	-9.60	7	37 °C	Cl, OH, NO3	543.9781
MS9-SARYD	6	10	50	2	102	2.04	19.335	24.4728	5.1378	300	5.58	92	58.6	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherical	Simulated Sweat	5.5	-9.60	7	37 °C	Cl, OH, NO3	593.1023
MS10-SARYD	7	10	50	2	108	2.16	19.5306	25.0028	5.4722	300	5.91	93	58.9	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherical	Simulated Sweat	5.5	-9.60	7	37 °C	Cl, OH, NO3	500.217

MS_Old	8	10	50	2	70	1.4	15.0442	17.239	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	Simulate	5.5	-9.60	7	37 °C	Cl, OH,	652.1281
MS_Old	9	10	50	2	70	1.4	15.0412	17.236	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	Simulate	5.5	-9.60	7	37 °C	Cl, OH,	621.1208
MS11-	10	10	50	2	108	2.16	19.3387	24.8853	5.5466	300	5.91	93	58.9	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	Simulate	5.5	-9.60	7	37 °C	Cl, OH,	524.0869
MS12-	11	10	50	2	108	2.16	19.2772	24.791	5.5138	300	5.91	94	59.7	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	Simulate	5.5	-9.60	7	37 °C	Cl, OH,	6.68594
MS 15-	12	10	50	2	108	2.16	19.1637	24.7323	5.5686	300	5.91	93	59.4	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	Simulate	5.5	-9.60	7	37 °C	Cl, OH,	750.608
Old 3-	13	10	50	2	70	1.4	15.0472	17.242	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	Simulate	5.5	-9.60	7	37 °C	Cl, OH,	7.827118
Old 7-	14	10	50	2	70	1.4	15.0412	17.236	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	Simulate	5.5	-9.60	7	37 °C	Cl, OH,	613.659

Old 8-	15	10	50	2	70	1.4	15.0412	17.236	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	Simulate	5.5	-9.60	7	37 °C	Cl, OH,	519.8772
Old 9-	16	10	50	2	70	1.4	15.0397	17.2345	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	Simulate	5.5	-9.60	7	37 °C	Cl, OH,	591.2169
Ni2	17		##	2	70	1.4	35.364	39.162	3.798	150	3.83	99	63.1	Aged	3	Ni	0	NA	300	35	NA	0	NA	NA	Simulate	5.5		7	37 °C	Cl, OH,	1026.541
Ni5	18	10	50	2	70	1.4	34.639	37.99	3.351	290	3.45	97	55.7	Aged	3	Ni coating	0	NA	300	35	NA	0	NA	NA	Simulated	5.5		7	37 °C	Cl, OH,	729.3549508
Ni6	19	10	50	2	70	1.4	35.1	38.85	3.75	300	3.83	98	62.3	Aged	3	Ni	0	NA	300	35	NA	0	NA	NA	Simulate	5.5		7	37 °C	Cl, OH,	813.4731
SAB	20	10	50	2	100	2	98.35	103.44	5.09	300	5.47	93	59.2	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	Simulate	5.5		7	37 °C	More N	1245.974
MS1-	1	10	50	1	70	0.7	17.4212	18.1545	0.7333	120	0.77	96	12.2	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	DMEM	7.2	-22.00	3	37 °C	More N	37.32328

MS3-SARYD	2	10	50	1	102	1.1	16.1352	16.6187	0.4835	120	1.2	40	5.5	Aged	3	Ni/SiC coatin	10	NA	300	35	NA	110	negative	Spherica	-	DMEM	7.2	-22.00	3	37 °C	More N after	336.7925
MS4-SARYD	3	10	50	2	102	2	16.4173	17.3072	0.8899	120	2.19	41	10.1	Aged	3	Ni/SiC coatin	10	NA	300	35	NA	110	negative	Spherica	-	DMEM	7.2	-22.00	3	37 °C	More N after	55.00438
MS7-SARYD	4	10	50	2	102	2	19.4487	23.572	4.1233	240	4.38	94	47	Aged	3	Ni/SiC coatin	10	NA	300	35	NA	110	negative	Spherica	-	DMEM	7.2	-22.00	3	37 °C	More N after	30.16481
MS8-SARYD	5	10	50	2	102	2	19.4828	23.524	4.0412	240	4.38	92	46.1	Aged	3	Ni/SiC coatin	10	NA	300	35	NA	110	negative	Spherica	-	DMEM	7.2	-22.00	3	37 °C	More N after	229.014
MS9-SARYD	6	10	50	2	102	2.04	19.335	24.4728	5.1378	300	5.58	92	58.6	Aged	3	Ni/SiC coatin	10	NA	300	35	NA	110	negative	Spherica	-	DMEM	7.2	-22.00	3	37 °C	More N after	249.7261
MS10-SARYD	7	10	50	2	108	2.16	19.5306	25.0028	5.4722	300	5.91	93	58.9	Aged	3	Ni/SiC coatin	10	NA	300	35	NA	110	negative	Spherica	-	DMEM	7.2	-22.00	3	37 °C	More N after	273.9498
MS_Old_2	8	10	50	2	70	1.4	15.0442	17.239	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC coatin	10	NA	300	35	NA	110	negative	Spherica	-	DMEM	7.2	-22.00	3	37 °C	More N after	9.488258

MS_Old 10	9	10	50	2	70	1.4	15.0412	17.236	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica	DMEM	7.2	-22.00	3	37 °C	More N after	22.06878
MS11-SARYD	10	10	50	2	108	2.16	19.3387	24.853	5.5466	300	5.91	93	58.9	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica	DMEM	7.2	-22.00	3	37 °C	More N after	241.2028
MS12-SARYD	11	10	50	2	108	2.16	19.2772	24.791	5.5138	300	5.91	94	59.7	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica	DMEM	7.2	-22.00	3	37 °C	More N after	267.4475
MS 15-SARYD	12	10	50	2	108	2.16	19.1637	24.7323	5.5686	300	5.91	93	59.4	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica	DMEM	7.2	-22.00	3	37 °C	More N after	317.3015
Old 3-conventi	13	10	50	2	70	1.4	15.0472	17.242	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica	DMEM	7.2	-22.00	3	37 °C	More N after	32.15947
Old 7-conventi	14	10	50	2	70	1.4	15.0412	17.236	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica	DMEM	7.2	-22.00	3	37 °C	More N after	27.80832
Old 8-conventi	15	10	50	2	70	1.4	15.0412	17.236	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC coating	10	NA	300	35	NA	110	negative	Spherica	DMEM	7.2	-22.00	3	37 °C	More N after	12.76705

Old 9-	16	10	50	2	70	1.4	15.0397	17.2345	2.1948	120	2.37	93	23.6	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	DMEM	7.2	-22.00	3	37 °C	More N	27.30003
Ni2	17		##	2	70	1.4	35.364	39.162	3.798	150	3.83	99	63.1	Aged	3	Ni	0	NA	300	35	NA	0	NA	NA	DMEM	7.2		3	37 °C	More N	388.2328
Ni5	18	10	50	2	70	1.4	34.639	37.99	3.351	290	3.45	97	55.7	Aged	3	Ni coating	0	NA	300	35	NA	0	NA	NA	DMEM	7.2		3	37 °C	More N after	26.00040151
Ni6	19	10	50	2	70	1.4	35.1	38.85	3.75	300	3.83	98	62.3	Aged	3	Ni	0	NA	300	35	NA	0	NA	NA	DMEM	7.2		3	37 °C	More N	34.16314
SABYD	20	10	50	2	100	2	98.35	103.44	5.09	300	5.47	93	59.2	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	ASW		-19.30	7	RT	NiO,	14.89097
SAB	20	10	50	2	100	2	98.35	103.44	5.09	300	5.47	93	59.2	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherica	WW		-7.15	7	RT	NiO,	19.40366
SABYDO	20	10	50	2	100	2	98.35	103.44	5.09	300	5.47	93	59.2	Aged	3	Ni/SiC	10	NA	300	35	NA	110	negative	Spherical	DMEM	7.2	-22.00	3	37 °C	NiO,	148.14867