SUPPORTING INFORMATION

Fe-doped ZnO nanoparticle toxicity: assessment by a new generation of nanodescriptors

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TABLE S1. Calculated nanodescriptors for Fe doped ZnO particles: Preliminary descriptors [*Nanoscale* **2016,** *8* (36), 16243].

#	Descriptor	Fe 0.00%	Fe 6.00%	Fe 10.00%
	Radius of NP (Å)	**82.5**	**51.5**	**47.0**
	Original descriptors (*See Tämm et. al.*[21])			
1	Log of total No. of atoms in NP.	5.2957	4.6817	4.5624
2	Log of total No. of atoms in core region of NP.	5.2196	4.5728	4.4516
3	Log of total No. of atoms in surface region of NP.	4.5019	4.1051	4.0351
4	Log of total No. of Zn atoms in NP.	4.9946	4.3414	4.1942
5	Log of total No. of Zn atoms in core region of NP.	4.9173	4.2102	4.0534
6	Log of total No. of Zn atoms in surface region of NP.	4.2073	3.7575	3.6366
7	Log of total No. of O atoms in NP.	4.9946	4.3807	4.2614
8	Log of total No. of O atoms in core region of NP.	4.9185	4.2536	4.1204
9	Log of total No. of O atoms in surface region of NP.	4.2009	3.7851	3.7042
10	Log of total No. of Fe atoms in NP.	0.0000	3.3179	3.4176
11	Log of total No. of Fe atoms in core region of NP.	0.0000	3.1872	3.2781
12	Log of total No. of Fe atoms in surface region of NP.	0.0000	2.7324	2.8567
13	Relative number of Fe atoms in NP	0.0000	0.0433	0.0717
14	Relative number of Fe atoms in core region of NP	0.0000	0.0412	0.0671
15	Relative number of Fe atoms in surface region of NP	0.0000	0.0424	0.0663
16	Avg. pot. energy of all atoms in NP in eV.	-18.8604	-18.5883	-18.4321
17	Avg. pot. energy of atoms in core region of NP in eV.	-18.9968	-18.7987	-18.6986
18	Avg. pot. energy of atoms in surface region of NP in eV.	-18.1528	-17.9773	-17.7366
19	Avg. pot. energy of Zn atoms in NP in eV.	-18.0444	-18.0844	-18.1258
20	Avg. pot. energy of Zn atoms in core region of NP in eV.	-18.1354	-18.2519	-18.3282
21	Avg. pot. energy of Zn atoms in surface region of NP in eV.	-17.5779	-17.6093	-17.5974
22	Avg. pot. energy of O atoms in NP in eV.	-19.6764	-19.2204	-18.9685
23	Avg. pot. energy of O atoms in core region of NP in eV.	-19.8732	-19.5248	-19.2962
24	Avg. pot. energy of O atoms in surface region of NP in eV.	-18.6489	-18.3261	-18.1141
25	Avg. pot. energy of Fe atoms in NP in eV.	N/A	-16.6037	-16.5201
26	Avg. pot. energy of Fe atoms in core region of NP in eV.	N/A	-16.8028	-16.7140
27	Avg. pot. energy of Fe atoms in surface region of NP in eV.	N/A	-16.0363	-16.0086
28	Avg. coordination No. of all atoms in NP.	3.9250	3.8863	3.8717
29	Avg. coordination No. of atoms in core region of NP.	4.0000	4.0000	4.0000
30	Avg. coordination No. of atoms in surface region of NP.	3.5370	3.7576	3.7455
31	Avg. coordination No. of Zn atoms in NP.	3.9250	3.8850	3.8719
32	Avg. coordination No. of Zn atoms in core region of NP.	4.0000	4.0000	4.0000
33	Avg. coordination No. of Zn atoms in surface region of NP.	3.5404	3.7544	3.7461
34	Avg. coordination No. of O atoms in NP.	3.9250	3.8863	3.8714
35	Avg. coordination No. of O atoms in core region of NP.	4.0000	4.0000	4.0000
36	Avg. coordination No. of O atoms in surface region of NP in.	3.5336	3.7571	3.7446
37	Avg. coordination No. of Fe atoms in NP.	N/A	3.9004	3.8716
38	Avg. coordination No. of Fe atoms in core region of NP.	N/A	4.0000	4.0000
39	Avg. coordination No. of Fe atoms in surface region of NP.	N/A	3.7950	3.7476
40	Diameter of the NP in Å.	165.6491	103.3880	94.3619
41	Surface area of the NP in Å2.	86204	33581	27973
42	Volume of the NP in Å3.	2379939	578640	439935
43	Lattice energy of NP in eV.	-37.7208	-37.1767	-36.8642
44	Relative lattice energy of NP to bulk material (eV)	-0.2765	-0.8206	-1.1331
45	Lattice energy of NP divided by the diameter of NP.	-1562.1043	-960.9059	-869.6438
46	Lattice energy of NP per unit surface area.	-0.0004	-0.0011	-0.0013

47	Lattice energy of NP per unit volume.	0.0000	-0.0001	-0.0001

Table S2. Calculated nanodescriptors for Fe doped ZnO particles: Newly developed descriptors.

#	Descriptor	Fe 0.00%	Fe 6.00%	Fe 10.00%
	Radius of NP (Å)	**82.5**	**51.5**	**47.0**
	Newly developed nanodescriptors			
48	Avg. length of force vector for all atoms	0.3010	0.3445	0.4652
49	Avg. length of force vector for all atoms in core region	0.2380	0.2665	0.3069
50	Avg. length of force vector for all atoms in surface region	0.6281	0.5710	0.8784
51	Avg. length of force vector for all Zn atoms	0.3064	0.5004	0.5634
52	Avg. length of force vector for Zn atoms in core region	0.2489	0.3973	0.4539
53	Avg. length of force vector for Zn atoms in surface region	0.6017	0.7927	0.8492
54	Avg. length of force vector for all O atoms	0.2060	0.2615	0.2754
55	Avg. length of force vector for O atoms in core region	0.2325	0.1979	0.2170
56	Avg. length of force vector for O atoms in surface region	0.6416	0.4358	0.6522
57	Avg. length of force vector for all Fe atoms	N/A	0.6913	1.6587
58	Avg. length of force vector for Fe atoms in core region	N/A	0.4860	0.6809
59	Avg. length of force vector for Fe atoms in surface region	N/A	1.2764	4.2385
60	Avg. length of force vector surface normal component for all atoms	0.0828	0.1031	0.0940
61	Avg. length of force vector surface normal component for all atoms in core region	0.0264	0.0256	0.0212
62	Avg. length of force vector surface normal component for all atoms in surface region	0.3752	0.3282	0.2838
63	Avg. length of force vector surface normal component for all Zn atoms	0.1381	0.2235	0.2213
64	Avg. length of force vector surface normal component for Zn atoms in core region	0.0580	0.0731	0.0646
65	Avg. length of force vector surface normal component for Zn atoms in surface region	0.5488	0.6502	0.6305
66	Avg. length of force vector surface normal component for all O atoms	0.0247	0.0606	0.0464
67	Avg. length of force vector surface normal component for O atoms in core region	0.0107	0.0040	0.0019
68	Avg. length of force vector surface normal component for O atoms in surface region	0.2871	0.1952	0.1683
69	Avg. length of force vector surface normal component for all Fe atoms	N/A	0.0013	-0.0261
70	Avg. length of force vector surface normal component for Fe atoms in core region	N/A	0.0298	0.0317
71	Avg. length of force vector surface normal component for Fe atoms in surface region	N/A	-0.0800	-0.1786
72	Avg. length of force vector surface tangent component for all atoms	0.2035	0.2375	0.3523
73	Avg. length of force vector surface tangent component for all atoms in core region	0.1810	0.2054	0.2393
74	Avg. length of force vector surface tangent component for all atoms in surface region	0.3203	0.3309	0.6471
75	Avg. length of force vector surface tangent component for all Zn atoms	0.1890	0.3222	0.3811
76	Avg. length of force vector surface tangent component for Zn atoms in core region	0.1818	0.3005	0.3502
77	Avg. length of force vector surface tangent component for Zn atoms in surface region	0.2257	0.3839	0.4617
78	Avg. length of force vector surface tangent component for all O atoms	0.1446	0.1890	0.2016
79	Avg. length of force vector surface tangent component for O atoms in core region	0.1806	0.1550	0.1708
80	Avg. length of force vector surface tangent component for O atoms in surface region	0.3487	0.1887	0.2384
81	Avg. length of force vector surface tangent component for all Fe atoms	N/A	0.5218	1.4392
82	Avg. length of force vector surface tangent component for Fe atoms in core region	N/A	0.3771	0.5312
83	Avg. length of force vector surface tangent component for Fe atoms in surface region	N/A	0.9340	3.8347
84	Avg. dipole moment of all O atoms (D)	0.1133	0.1028	0.1289
85	Avg. dipole moment of O atoms in core region (D)	0.0530	0.0618	0.0814
86	Avg. dipole moment of O atoms in surface region (D)	0.1736	0.1437	0.1763

Table S3. Experimental values of biological endpoints (unitless), doping amount and radii for modeled NPs.

Biological endpoint		Cell death		Membrane damage		Mitochondrial ROS	
Doping (weight%)	**Radius(Å)**	**HeLa**	**KLN205**	**HeLa**	**KLN205**	**HeLa**	**KLN205**
0% Fe	82,5	2,174	2,326	2,840	2,990	4,210	4,440
1% Fe	72,5	1,754	1,887	2,330	2,460	3,760	3,720
2% Fe	64,0	1,613	1,724	2,180	2,260	3,460	3,670
4% Fe	53,0	1,351	1,408	1,630	1,720	2,780	2,830
6% Fe	51,5	1,299	1,316	1,540	1,620	2,340	2,390
8% Fe	50,0	1,250	1,220	1,550	1,490	2,210	2,310
10% Fe	47,0	1,205	1,266	1,430	1,540	2,160	2,170

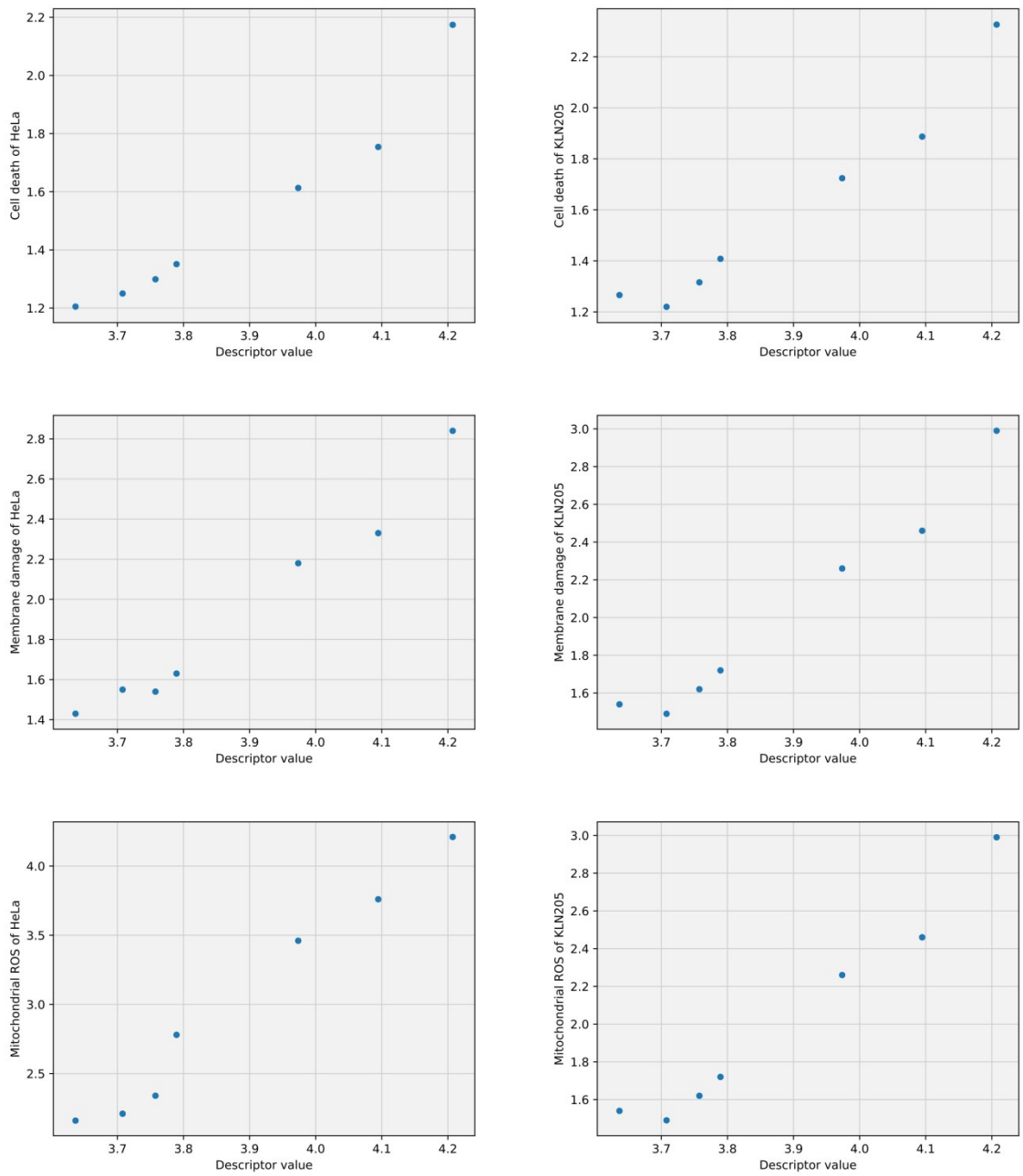

Figure S1. Plots of biological endpoints vs. *The log number of Zn atoms in shell region of NP*.

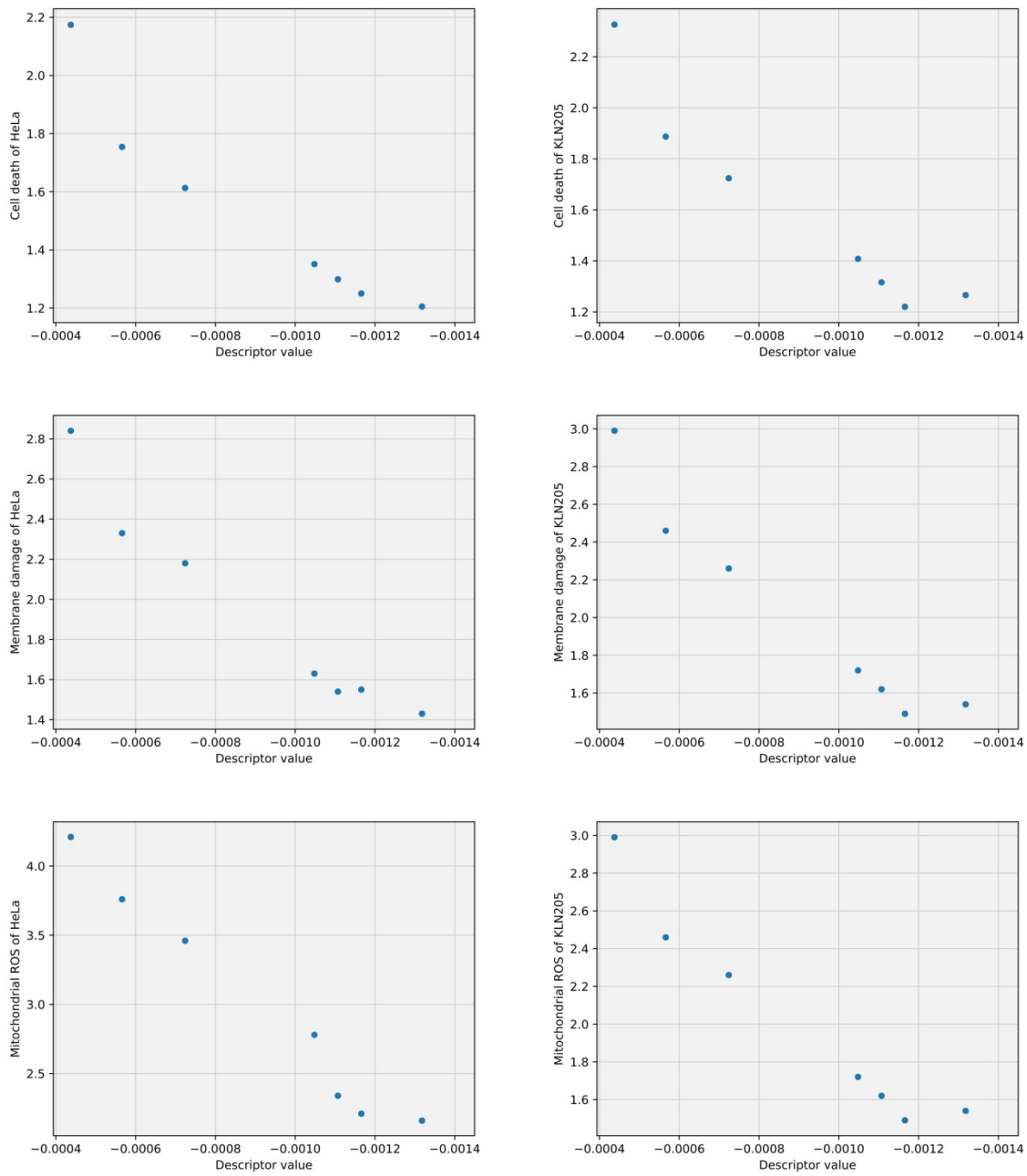

Figure S2. Plots of biological endpoints vs. *The lattice energy of NP/Surface area of NP*.

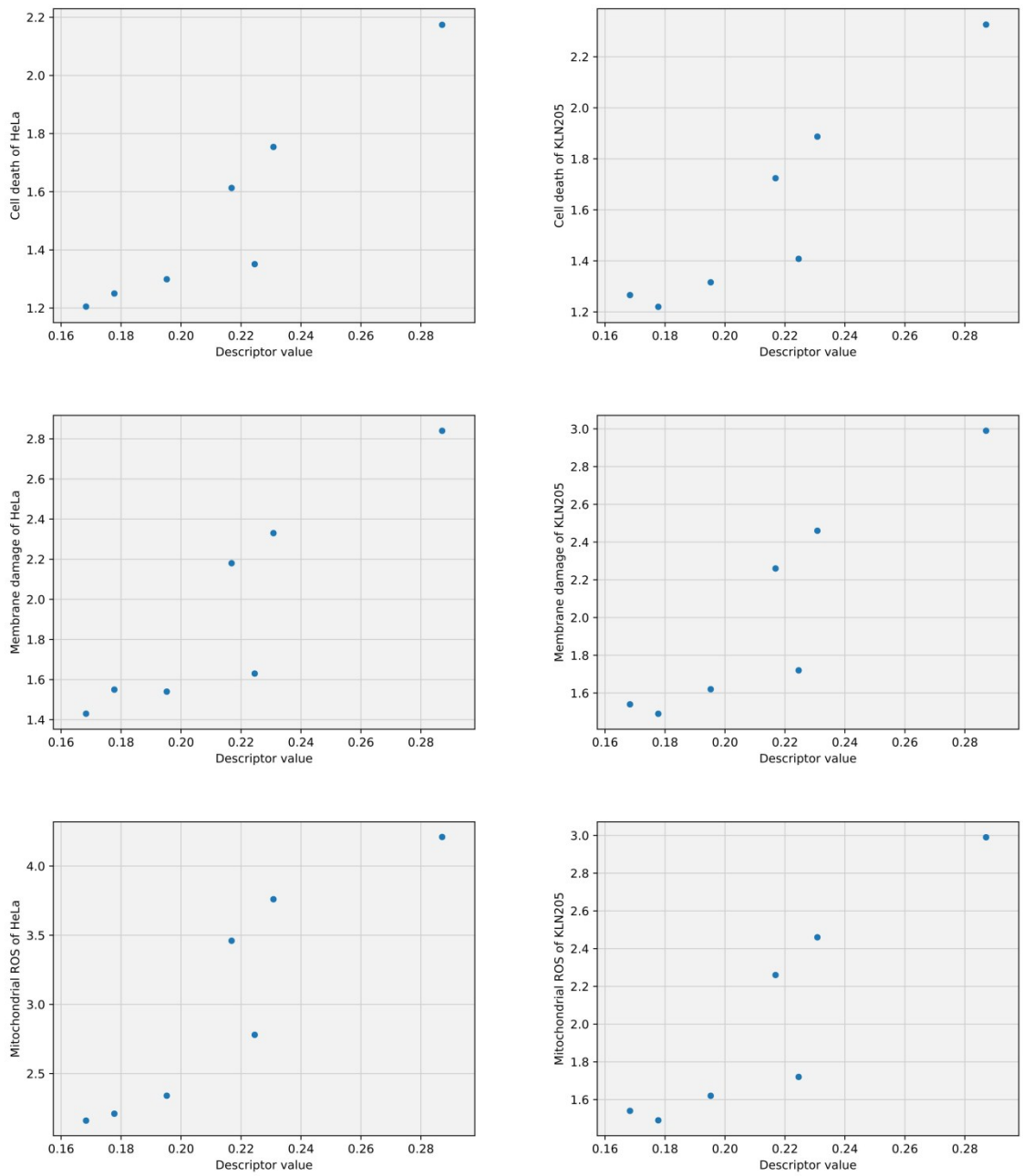

Figure S3. Plots of biological endpoints vs. *The average force vector surface normal component of oxygen atoms in shell region*.