ELECTRONIC SUPPLEMENTARY INFORMATION

Impact of Speciation on the Electron Charge Transfer Properties of Nanodiamond Drug Carriers

B. Sun and A. S. Barnard*

CSIRO Virtual Nanoscience Laboratory, 343 Royal Parade, Parkville 3052, Victoria, Australia

E-mail: amanda.barnard@csiro.au

*To whom correspondence should be addressed

Thermodynamically Limited Boltzmann Distribution

Table 1: Boltzmann distribution, for samples that are thermodynamically limited: Shapes, with the probability distributed over all sizes.

	Expectation Values (eV)				Quality Factors (arb.)			
	IP	EA	E_{gap}	E_{Fermi}	IP	EA	E_{gap}	E_{Fermi}
Octahedron	5.063	4.153	0.910	-4.611	33.0	24.4	3.0	86.4
Rhombi-truncated Octahedron	5.380	4.569	0.810	-4.973	28.2	26.5	3.0	39.6
Truncated Octahedron	5.306	4.413	0.892	-4.859	47.6	23.0	3.9	44.9
Doubly-truncated Octahedron	5.145	4.337	0.808	-4.755	28.5	18.4	2.3	41.6
Rhombic Dodecahedron	5.614	4.823	0.791	-5.215	37.8	29.3	5.2	37.2
Truncated Dodecahedron	5.748	4.889	0.859	-5.320	33.4	21.7	6.1	28.1
Small Rhombicuboctahedron	5.458	4.497	0.961	-4.975	35.0	21.5	4.6	32.1
Doubly-truncated Dodecahedron	5.576	4.755	0.820	-5.164	37.7	17.0	2.9	30.4
Cube	6.052	5.060	0.991	-5.558	15.1	16.9	4.6	16.2
Truncated Cube	5.674	4.851	0.823	-5.262	36.2	31.3	3.2	58.7
Cuboctahedron	5.488	4.760	0.729	-5.096	24.2	16.0	4.7	31.8
Great Rhombicuboctahedron	5.570	4.630	0.940	-5.100	144.9	29.9	29.2	34.1
Mixture (All)	5.442	4.583	0.859	-5.012	18.9	14.6	3.3	18.9

Table 2: Boltzmann distribution, for samples that are thermodynamically limited: Facet-constrained samples, with the probability distributed over all sizes.

	Expectation Values (eV)				Quality Factors (arb.)			
	IP	EA	E_{gap}	E_{Fermi}	IP	EA	E_{gap}	E_{Fermi}
(111)-enriched	5.230	4.379	0.852	-4.809	25.9	18.1	2.9	29.2
(110)-enriched	5.582	4.710	0.873	-5.144	29.3	17.1	4.0	24.2
(100)-enriched	5.623	4.772	0.851	-5.188	22.1	17.8	3.7	22.1
Quasi-spherical	5.449	4.582	0.866	-5.018	21.0	16.4	3.2	21.7
Highly facetted	5.433	4.585	0.848	-5.004	16.8	12.8	3.5	16.3

Table 3: Boltzmann distribution, for samples that are thermodynamically limited: Speciation-constrained samples, with the probability distributed over all sizes.

	Expectation Values (eV)				Quality Factors (arb.)			
	IP	EA	E_{gap}	E_{Fermi}	IP	EA	E_{gap}	E_{Fermi}
sp^3-enriched	5.563	4.727	0.837	-5.148	24.1	18.4	4.6	23.1
sp^2-enriched	5.265	4.374	0.891	-4.822	24.7	19.8	3.0	30.4
sp^{2+x}-enriched	5.515	4.663	0.852	-5.082	18.5	14.8	2.7	20.3
$N_{coord} < 3.5$	5.221	4.253	0.967	-4.737	22.0	19.7	3.3	27.8
$N_{coord} > 3.5$	5.509	4.683	0.826	-5.095	20.5	17.4	3.5	22.0

Size-dependent Normal Distribution

Table 4: Normal distribution, for samples that are kinetically limited: Shapes, with the probability distributed over all sizes.

	Expectation Values (eV)				Quality Factors (arb.)			
	IP	EA	E_{gap}	E_{Fermi}	IP	EA	E_{gap}	E_{Fermi}
Octahedron	5.030	4.144	0.886	-4.589	32.1	27.4	3.0	101.9
Rhombi-truncated Octahedron	5.379	4.573	0.805	-4.977	26.1	23.3	2.8	34.8
Truncated Octahedron	5.311	4.350	0.961	-4.830	40.4	31.0	5.2	48.4
Doubly-truncated Octahedron	5.121	4.394	0.727	-4.761	25.3	20.7	2.0	45.7
Rhombic Dodecahedron	5.590	4.801	0.789	-5.190	34.5	25.5	4.8	32.9
Truncated Dodecahedron	5.755	4.870	0.884	-5.315	34.3	21.2	5.6	28.2
Small Rbombicuboctahedron	5.496	4.495	1.001	-4.994	35.1	20.4	5.2	29.9
Doubly-truncated Dodecahedron	5.583	4.773	0.811	-5.176	41.4	13.9	2.3	27.0
Cube	6.104	5.114	0.990	-5.611	15.7	16.4	4.7	16.5
Truncated Cube	5.681	4.849	0.832	-5.265	34.1	29.9	3.1	54.8
Cuboctahedron	5.430	4.716	0.714	-5.042	23.7	15.6	4.1	35.1
Great Rhombicuboctahedron	5.571	4.623	0.948	-5.096	178.6	30.8	33.2	34.6
Mixture (All)	5.464	4.601	0.863	-5.030	17.4	14.4	3.2	17.9

Table 5: Normal distribution, for samples that are kinetically limited: Facet-constrained, with the probability distributed over all sizes.

	Expectation Values (eV)				Quality Factors (arb.)			
	IP	EA	E_{gap}	E_{Fermi}	IP	EA	E_{gap}	E_{Fermi}
(111)-enriched	5.225	4.388	0.837	-4.808	23.4	19.3	2.8	28.5
(110)-enriched	5.595	4.708	0.887	-5.150	30.4	16.2	3.8	23.9
(100)-enriched	5.644	4.776	0.868	-5.203	20.1	17.2	3.6	20.1
Quasi-spherical	5.457	4.594	0.863	-5.026	20.1	17.0	3.0	21.8
Highly facetted	5.472	4.609	0.863	-5.035	15.1	12.3	3.6	14.9

Table 6: Normal distribution, for samples that are kinetically limited: Speciation-constrained, with the probability distributed over all sizes.

	Expectation Values (eV)				Quality Factors (arb.)			
	IP	EA	E_{gap}	E_{Fermi}	IP	EA	E_{gap}	E_{Fermi}
sp^3-enriched	5.589	4.726	0.863	-5.159	25.9	18.7	5.0	23.8
sp^2-enriched	5.251	4.387	0.863	-4.820	26.0	25.7	3.5	34.5
sp^{2+x}-enriched	5.556	4.727	0.830	-5.140	20.3	19.0	3.0	23.5
$N_{coord} < 3.5$	5.205	4.272	0.934	-4.738	21.8	21.9	3.3	29.0
$N_{coord} > 3.5$	5.537	4.693	0.843	-5.113	18.8	16.5	3.2	20.3

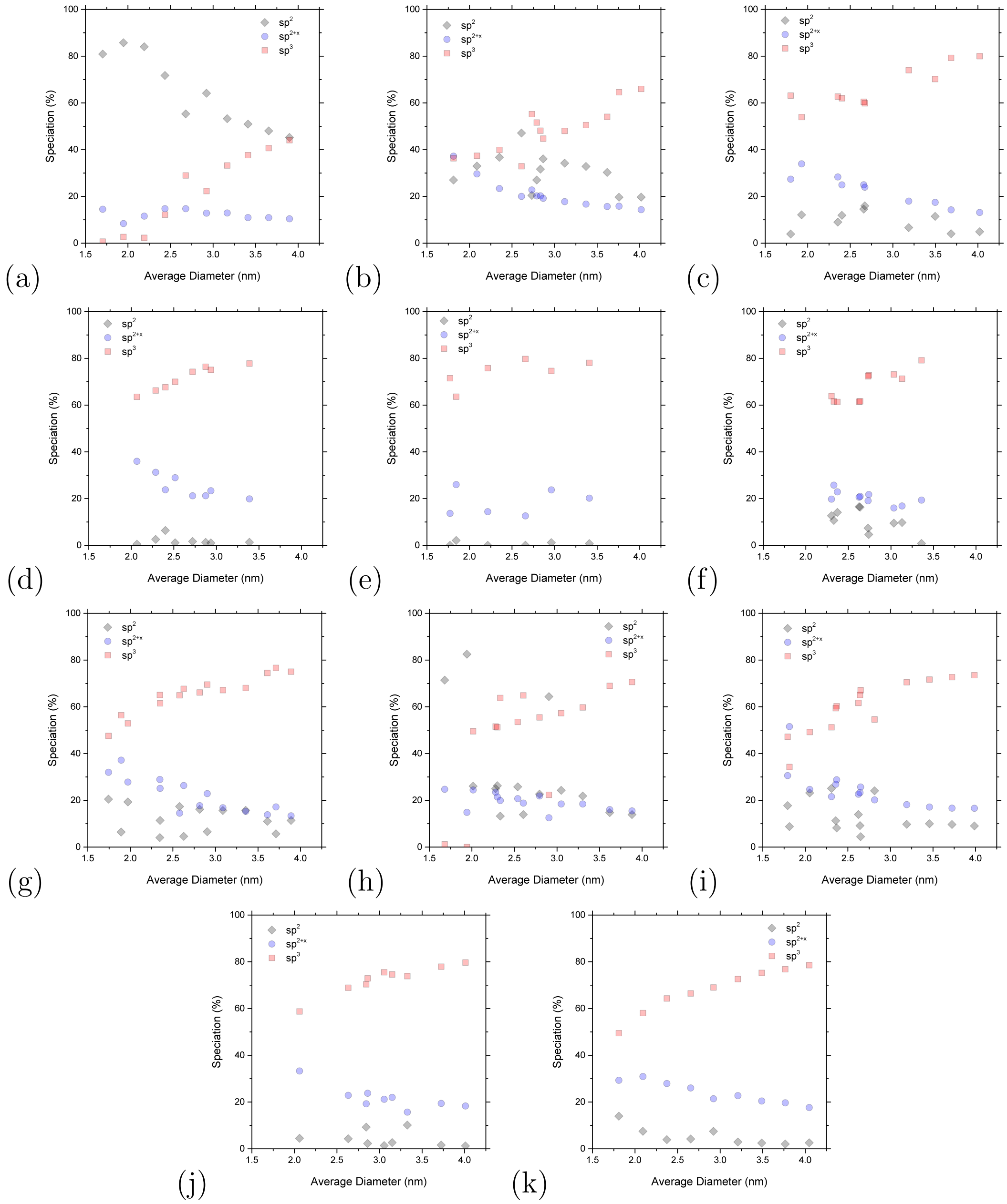


Figure 1: Size-dependent speciation for each of the shapes represented in the dataset used in this study: (a) the octahedron, (b) truncated octahedron, (c) cuboctahedron, (d) truncated cube, (e) cube, (f) great rhombicuboctahedron, (g) small rhombicuboctahedron, (h) doubly-truncated octahedron, (i) rhombi-truncated octahedron, (j) truncated dodecahedron and (k) the rhombic dodecahedron.

Bond Length Distributions

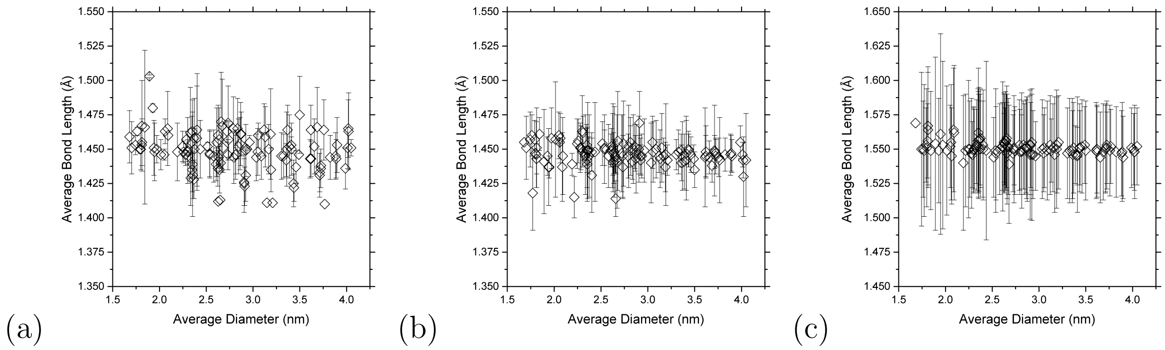


Figure 2: Bond lengths, with error bar representing the bond length distribution, for each bucky-diamond structure represented in this dataset, separated according to the speciation: (a) sp^2 hybridized atoms, (b) sp^{2+x} hybridized atoms, and (c) sp^3 hybridized atoms.

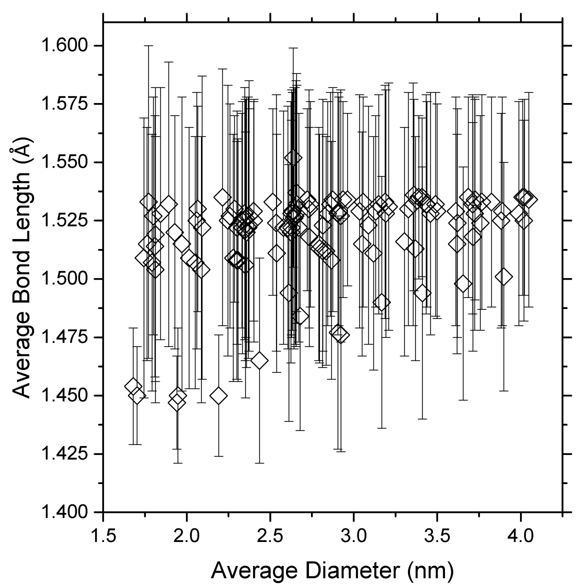
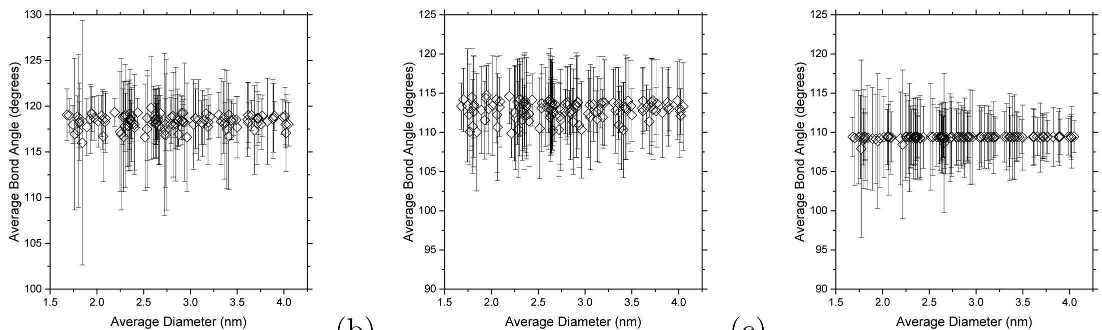


Figure 3: The average bond length, with error bar representing the bond length distribution, for each of the bucky-diamond structure represented in this dataset, averaging over all bond types.

Bond Angle Distributions



(a) (b) (c)

Figure 4: Bond angles, with error bar representing the bond length distribution, for each bucky-diamond structure represented in this dataset, separated according to the speciation: (a) sp^2 hybridized atoms, (b) sp^{2+x} hybridized atoms, and (c) sp^3 hybridized atoms.

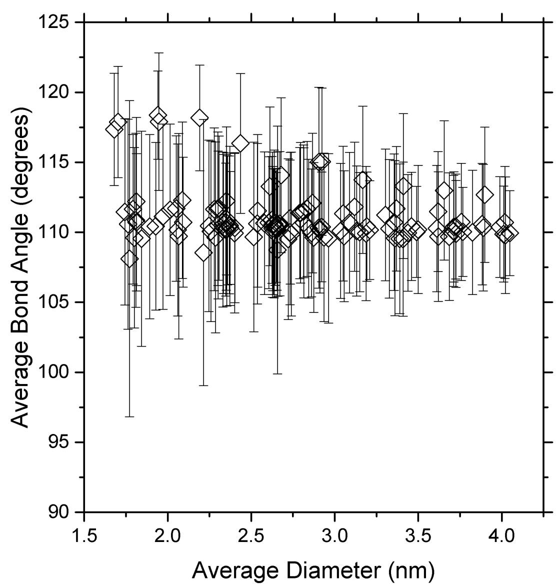


Figure 5: The average bond angle, with error bar representing the bond length distribution, for each of the bucky-diamond structure represented in this dataset, averaging over all bond types.

Acknowledgement

Computational resources for this project were supplied by the National Computational Infrastructure national facility under Partner Allocation Scheme, Grant q27.