Supporting Material

Structural and Magnetic Properties of $Gd_3N@C_{80}$

Jing Lu,*[†,‡] Renat F. Sabirianov,[‡,§] Wai Ning Mei,[‡,§] Yi Gao,[§,∥] Chungang Duan,[⊥] and Xiaocheng Zeng[§,∥]

[†]Mesoscopic Physics Laboratory, Department of Physics, Peking University, Beijing 100871, P. R. China.
[‡]Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182-0266, USA.
[§]Nebraska Center for Material and Nanoscience, University of Nebraska at Lincoln, Lincoln, Nebraska, 68588, USA.
[∥]Department of Chemistry, University of Nebraska at Lincoln, Lincoln, Nebraska 68588, USA.
[⊥]Department of Physics, University of Nebraska at Lincoln, Lincoln, Nebraska 68588,USA.

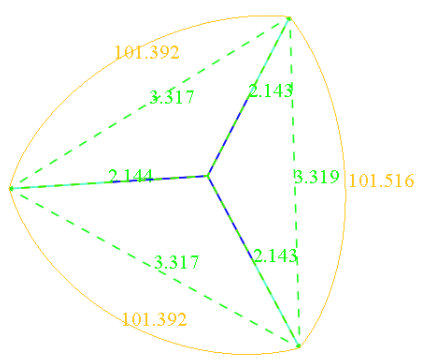

Fig.S1. Visualized structure parameters of an optimized free-standing Gd_3N cluster.

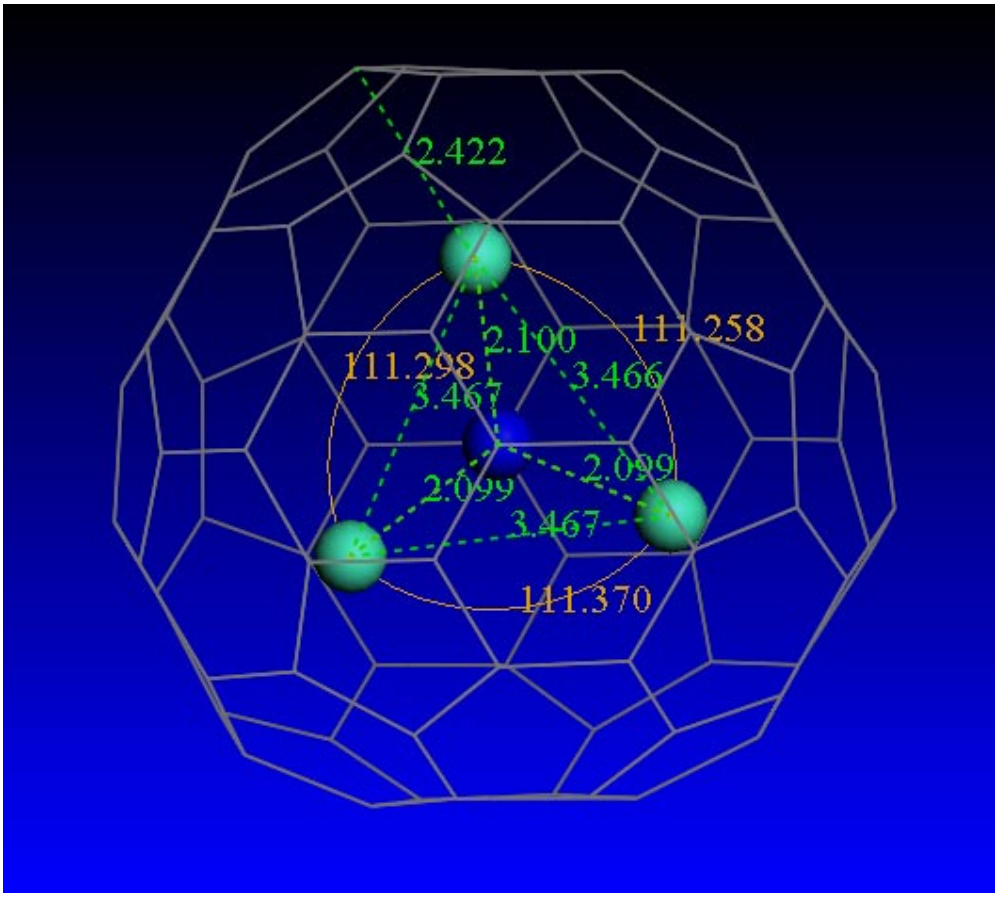

Fig.S2. Visualized structure parameters of $Gd_3N@C_{80}$ (II).

Coordinates (Angstroms) of $Gd_3N@C_{80}$ (II)

	ATOM	X	Y	Z
1	Gd	19.353915	7.502898	1.071103
2	N	17.999554	7.507936	2.674564
3	Gd	16.987338	9.341831	2.814041
4	Gd	16.650830	5.903480	2.538001
5	C	18.072291	5.305373	5.552276
6	C	17.066467	6.226392	5.950023
7	C	17.459613	7.567738	6.254780
8	C	15.754824	6.010967	5.421878
9	C	17.784355	4.256375	4.594743
10	C	16.372992	3.502518	2.690774
11	C	16.461747	3.988691	4.075472

12	C	15.428357	4.911907	4.523293
13	C	14.918408	7.134697	5.113580
14	C	15.339714	8.488190	5.355936
15	C	16.602234	8.681332	5.964369
16	C	14.872139	9.531521	4.474508
17	C	14.108312	6.778900	3.987607
18	C	13.615436	7.381501	1.697498
19	C	13.736150	7.786518	3.046557
20	C	14.112531	9.154602	3.316445
21	C	15.310933	3.996502	1.771593
22	C	14.325986	4.986361	2.222592
23	C	14.382215	5.398266	3.614653
24	C	13.965225	6.030965	1.293334
25	C	15.602169	10.768949	4.193601
26	C	16.965328	10.885533	4.732595
27	C	17.419764	9.826768	5.606384
28	C	17.984136	11.430193	3.846026
29	C	15.303021	11.125290	2.779445
30	C	16.345252	11.113456	0.522181
31	C	16.362723	11.599299	1.881834
32	C	17.687037	11.780513	2.451263
33	C	13.942740	8.291120	0.635695
34	C	14.385751	9.625792	0.903762
35	C	14.399965	10.094888	2.269290
36	C	15.351887	10.186189	0.025690
37	C	19.344463	10.909381	3.872839
38	C	19.773292	9.886093	4.775129
39	C	18.796677	9.379130	5.674294
40	C	20.828128	9.014753	4.358850
41	C	19.895466	10.967057	2.550106
42	C	20.932685	9.660237	0.712610
43	C	20.903725	10.043684	2.104238
44	C	21.386652	9.098356	3.039147
45	C	17.545088	10.877252	-0.261679
46	C	18.826847	10.995961	0.323919
47	C	18.875360	11.458819	1.674016
48	C	19.869724	10.111280	-0.139381
49	C	20.842367	7.636015	4.753132
50	C	19.806602	7.099670	5.576296
51	C	18.814428	7.999745	6.070862
52	C	19.427338	5.739277	5.367221
53	C	21.417692	6.869468	3.684829
54	C	20.964001	5.135722	2.049690
55	C	20.970220	5.547507	3.419524

56	C	20.004768	4.970997	4.303345
57	C	21.441525	8.381350	0.215101
58	C	21.810538	7.367686	1.214241
59	C	21.770310	7.767248	2.603241
60	C	21.390880	5.997749	0.956232
61	C	19.940191	4.249767	1.576932
62	C	18.925767	3.724740	2.450223
63	C	18.998754	4.068666	3.820294
64	C	17.612089	3.460997	1.912073
65	C	19.669703	4.584963	0.210999
66	C	17.930465	5.366541	-1.279902
67	C	18.344791	4.434472	-0.300143
68	C	17.337526	3.859079	0.560463
69	C	20.611882	8.024454	-0.968099
70	C	18.783875	6.482661	-1.649594
71	C	20.134382	6.650495	-1.166755
72	C	20.572416	5.647152	-0.211118
73	C	17.282341	9.848040	-1.227997
74	C	17.899516	7.593378	-1.926866
75	C	18.298353	8.925702	-1.635505
76	C	19.641883	9.104904	-1.138735
77	C	14.514936	7.522625	-0.434112
78	C	16.540013	7.162397	-1.749181
79	C	15.543982	8.060763	-1.262307
80	C	15.924776	9.418339	-1.045894
81	C	15.950671	4.224523	0.477058
82	C	16.557174	5.783161	-1.348797
83	C	15.571513	5.265263	-0.448988
84	C	14.535887	6.143030	-0.031242