

Doped golden fullerene cages: Supporting Material

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In the following, we are reporting the xyz-coordinate files of few relaxed structures considered in our work "Doped golden fullerene cages". In particular, here we are reporting four shapes, two lump and two hollow for Au-pure cases. We also provide the Worm-like coordinate for Ag and Cu, as the Worm-like shows different relaxations in the three metals.

ATOMIC_POSITIONS (angstrom) golden fullerene			ATOMIC_POSITIONS (angstrom) Worm-like			
Au	3.51022363	0.486307353	Au	12.341312471	5.095928065	6.118169684
Au	6.56292963	-2.82301331	Au	7.531779564	0.795376107	2.948180868
Au	3.47220278	-7.53409529	Au	10.211777272	1.349621944	2.363103967
Au	5.54843807	-7.09310150	Au	3.956202855	1.417146379	6.134469514
Au	5.11316729	-0.62531197	Au	11.735148874	5.950060629	3.453439259
Au	7.20402718	-6.17637253	Au	2.916449625	3.975222773	6.107234242
Au	9.12224579	-4.49848318	Au	5.551461890	2.844092371	2.567669711
Au	7.85413742	-6.25477886	Au	7.314970699	7.907318238	3.091065811
Au	7.79122877	-0.96215862	Au	3.670243662	4.908062175	2.671916819
Au	2.19470549	-2.15093255	Au	10.922302027	3.965068223	1.731285212
Au	4.49593687	-6.96654606	Au	9.129432995	5.983334788	2.160724623
Au	1.81906474	-6.62973547	Au	6.383835561	5.418721670	2.170266004
Au	4.06330109	-0.49935803	Au	11.165973701	7.536344685	5.790845031
Au	3.94848561	-2.36061120	Au	5.424449621	3.504808421	7.257015856
Au	6.10007381	-8.07942772	Au	9.772132426	5.561560190	7.188798067
Au	8.21916008	-1.90827453	Au	8.242639149	3.385461763	2.143955092
Au	7.42975855	-3.48960733	Au	10.019271055	8.228840242	3.394075590
Au	1.39191127	-5.68482161	Au	9.274024413	1.938584076	4.876849850
Au	7.41577864	-5.44193268	Au	3.012975104	2.495476844	3.706260060
Au	4.74894905	-4.97155476	Au	8.157028966	3.306588298	7.064616007
Au	2.18136501	-4.10143328	Au	11.798472555	3.051389195	4.194708302
Au	6.70863390	-0.83384311	Au	8.415218556	7.579405430	5.698008958
Au	6.13845587	-5.953815E-02	Au	5.685248625	7.398798817	5.347312442
Au	1.75596106	-1.33733535	Au	7.008931668	5.809379692	7.289816125
Au	0.48834953	-3.09455514	Au	1.027823116	4.585564485	4.155766768
Au	1.12950397	-3.97689199	Au	14.217521996	4.607436600	4.184125064
Au	2.90274119	-6.75857973	Au	10.855826545	2.959274196	6.866532401
Au	4.86039352	-2.62023807	Au	4.611386024	7.508386387	2.743991776
Au	5.66333914	-5.23160982	Au	3.066700209	6.504159063	4.862091133
Au	8.48070717	-3.61531305	Au	4.897588004	0.393254398	3.659826654
Au	2.40585804	-1.41610956	Au	4.278424061	6.025611910	7.321632911
Au	3.04800773	-4.76995230	Au	6.624965202	1.598391843	5.542956299

ATOMIC_POSITIONS (angstrom) incomplete Dh

Au	-1.244763197	0.149234823	3.843812240
Au	5.138222971	2.434796596	5.686670025
Au	1.232927658	0.329114642	2.605707419
Au	-2.314457089	2.216602705	7.195619440
Au	-1.521336323	4.266734882	8.899042813
Au	-0.423454557	2.623389918	2.515664022
Au	-0.692999470	6.780630984	7.593000104
Au	-2.521533279	2.745355206	4.395245797
Au	1.263109719	-0.668030079	5.155881808
Au	-0.909015508	4.969126614	3.914569050
Au	2.164038328	1.168732345	10.071845781
Au	2.879024861	3.984801446	9.694569947
Au	1.708718201	2.277025075	7.602141664
Au	0.332189696	4.426936037	6.628492672
Au	2.260227022	2.780709724	1.896054582
Au	2.767828016	0.028106356	9.515526441
Au	-0.570964305	1.222045871	3.510267853
Au	-3.523867789	-2.838911005	7.988833166
Au	-3.145180628	1.839641958	7.334735225
Au	-5.688953250	2.271480104	8.431958515
Au	-1.367366500	1.030391941	11.695627485
Au	0.899883450	3.809624135	5.991763921
Au	-1.714091968	-2.939147764	5.553490923
Au	-2.541626533	-1.028806549	10.024006470
Au	-3.675798561	4.125843829	9.019188928
Au	0.278805373	-0.912787586	10.612208470
Au	-4.397890965	3.856384765	6.098837488
Au	1.171509596	2.144450759	10.453719136
Au	0.640712987	-0.512091135	7.689988683
Au	-1.407536723	4.287068034	7.473478094
Au	-3.189655544	1.158816958	4.436496527
Au	1.932699387	-2.593132394	9.051920198
Au	-3.690099720	1.574175100	10.292671781

ATOMIC_POSITIONS (angstrom) polyIh

Au	4.439406941	2.018798294	8.418833640
Au	1.680376366	5.189107726	3.061203344
Au	0.333922714	3.177597498	10.631825735
Au	-1.142353269	-0.234070742	6.652100586
Au	0.072574285	2.025162513	5.353287811
Au	4.232404799	4.585437972	7.350385612
Au	-2.474828186	4.857655374	6.314768055
Au	1.436222835	-0.567917942	7.960094850
Au	2.243697712	6.459122764	7.542346577
Au	3.549307187	0.241614534	6.354472217
Au	4.348038652	3.941666059	3.309349567
Au	0.735022945	6.844061706	5.132739543
Au	3.638578721	1.104817357	3.710520127
Au	0.749072344	5.737310837	9.720854493
Au	-0.595430333	1.149022617	9.038976683
Au	2.467601292	3.340257386	5.207918675
Au	3.531955428	6.011709678	5.082804752

ATOMIC_POSITIONS (angstrom)	Worm-like	Cu	8.96784401	2.09106159	5.00722265
Ag 12.3918524	4.92374134	6.29674006	Cu 3.40737438	2.94350266	3.50554013
Ag 7.53362036	0.97272295	2.87785006	Cu 7.93350744	3.37036443	6.80428076
Ag 10.2427759	1.33676946	2.50765896	Cu 11.3683929	2.47986698	4.65059662
Ag 4.01140308	1.59547997	6.04615831	Cu 8.44282532	6.78058004	5.14717102
Ag 11.4911194	5.78250933	3.73952985	Cu 5.92253542	6.79262447	5.01466799
Ag 2.98854494	4.22034216	5.88599491	Cu 7.03906059	5.65798903	6.91265774
Ag 5.49836540	2.87813783	2.32584262	Cu 1.83977449	4.78754044	3.86671138
Ag 7.43785572	8.06325150	2.85731912	Cu 13.1386795	4.11770725	3.98470616
Ag 3.63559866	4.99510384	2.62061453	Cu 10.3464737	2.96715522	6.91415691
Ag 10.9956512	3.90698004	1.73840261	Cu 5.02972317	7.43408918	2.84917140
Ag 9.21881008	6.05441332	1.98379564	Cu 3.49050355	6.54366302	4.66007757
Ag 6.45842028	5.40090990	2.86870790	Cu 5.00899029	1.05614400	3.50094199
Ag 10.9766178	7.39064837	5.99488544	Cu 4.52852392	6.02467680	6.91208029
Ag 5.28348351	3.64521241	7.42470598	Cu 6.51869059	2.24146485	5.12435961
Ag 9.80886745	5.28315258	7.30533981			
Ag 8.57538795	3.62020659	3.22129488			
Ag 10.2010174	8.29262733	3.45933414			
Ag 9.20431709	1.69351172	5.14473248			
Ag 2.97194004	2.54732132	3.62172484			
Ag 8.05454063	3.12364340	7.28732967			
Ag 11.6171341	2.98792934	4.37950563			
Ag 8.59113503	6.24676132	4.78708220			
Ag 5.80133200	7.15421247	5.02539539			
Ag 7.06376553	5.77589417	7.13639021			
Ag 0.98386079	4.73603630	4.00731611			
Ag 14.0685196	4.50639296	4.11525726			
Ag 10.8663130	2.72443700	7.13897371			
Ag 4.64873743	7.57821751	2.49986362			
Ag 2.98872185	6.77755880	4.68575382			
Ag 4.89401865	0.46989575	3.62992597			
Ag 4.27900982	6.29142094	7.18796921			
Ag 6.43878222	2.61322808	5.00531530			

ATOMIC_POSITIONS (angstrom)	Worm-like
Cu 11.6202841	4.66237831 5.77556562
Cu 7.44074345	1.21052921 3.10389328
Cu 9.94897366	1.48487294 2.84773874
Cu 4.14121532	1.96382642 5.65662909
Cu 11.4962940	5.92986917 3.62066698
Cu 3.37938523	4.26576328 5.64744997
Cu 5.80605173	3.22422266 2.85815859
Cu 7.53789425	7.79816389 3.11122370
Cu 4.24048042	5.12452078 2.86594510
Cu 10.7327490	3.86044455 2.73818159
Cu 9.10513115	5.77678442 2.96192980
Cu 6.67047215	5.50822878 2.99116468
Cu 10.8442659	7.03910255 5.66898775
Cu 5.50655365	3.74775290 6.80021191
Cu 9.47489929	5.27202749 6.80482864
Cu 8.31154251	3.48870111 2.99660754
Cu 9.98168945	7.94305086 3.50318527