Electronic Supplementary Information for:

Global minimization of gold clusters by combining neural network potentials and the basin-hopping method

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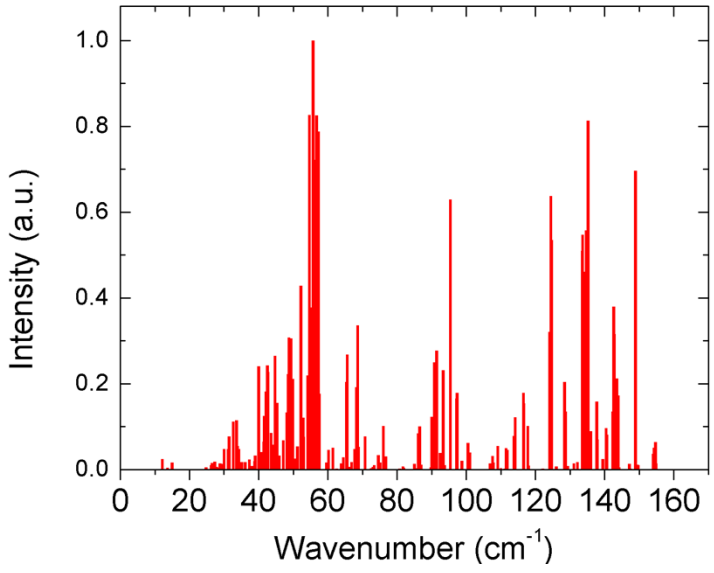
Figure S1. Simulated IR spectrum of Au_{58} isomer a (Figure 5 in the main text; forces converged to 0.001 eV/angstrom; see below for their coordinates) based on density-functional perturbation theory [D. Karhánek, T. Bučko, J. Hafner, J. Phys.: Condens. Matter 22 265006 (2010)].



XYZ coordinates in angstrom:

Au_{58} structure 1: Isomer (a) from this work (Figure 5): forces converged to 0.001 eV/angstrom

Au	4.148416	4.631794	5.709146
Au	6.173530	4.293007	10.696283
Au	6.129020	4.548720	7.760482
Au	8.282126	5.909572	6.673260
Au	8.654445	4.270250	9.485034
Au	9.115306	2.834631	7.157181
Au	4.193251	2.853186	9.338163
Au	3.718424	5.949770	8.163898
Au	7.052181	1.296246	6.206949
Au	4.767602	0.793766	7.644937
Au	6.932875	2.135165	8.891042
Au	10.957384	4.769395	8.068108
Au	8.034117	6.321074	11.236433
Au	2.275264	3.258288	4.178861
Au	2.997028	5.157489	2.226946
Au	0.793766	5.643544	3.790784
Au	5.362479	6.271804	3.666117
Au	6.747207	4.003294	4.993088
Au	8.168045	6.158144	3.869227
Au	4.416345	1.653443	5.036490
Au	5.598144	5.165617	1.037312
Au	7.467157	3.355809	2.105033
Au	10.026813	4.293095	2.672640
Au	9.002228	2.344352	4.402302
Au	4.716128	3.067587	2.670380
Au	6.624097	1.153950	3.477582
Au	8.336097	5.757314	1.006091
Au	10.622175	4.427155	5.382781
Au	2.449718	7.806993	3.297102
Au	2.923027	9.881840	5.135018
Au	6.898643	8.183990	5.354682
Au	3.960064	7.454434	1.026559
Au	11.008102	6.666802	3.768814
Au	6.619826	7.905165	1.435038
Au	7.465599	9.950270	3.172473
Au	5.571087	10.841403	5.120240
Au	9.311445	8.134907	2.098770
Au	4.741222	9.336341	2.980175
Au	9.765143	8.966909	4.717690
Au	2.607423	2.448277	6.962100
Au	3.508891	5.075256	10.907079
Au	1.199319	4.788075	6.351174
Au	1.701320	4.087279	9.024952
Au	0.951062	6.699502	8.376756
Au	2.454001	9.010835	7.822741

Au	2.760793	7.680826	10.261186
Au	1.201286	7.608678	5.752395
Au	4.143213	7.481402	5.836911
Au	9.127946	9.108516	7.462447
Au	6.121938	7.396602	7.892161
Au	6.696535	10.411196	7.767269
Au	5.448959	7.083923	10.813726
Au	9.641863	6.973514	9.106973
Au	8.282133	11.073826	5.622504
Au	4.765977	9.455066	9.493788
Au	10.871508	7.123555	6.530625
Au	4.062190	11.172008	7.390331
Au	7.577894	8.744814	9.847538

Au_{58} structure 2: Isomer (a) from this work (Figure 5): forces converged to 0.03 eV/angstrom

Au	4.149865	4.652486	5.675709
Au	6.174347	4.297151	10.688696
Au	6.104101	4.528078	7.746674
Au	8.279789	5.873981	6.668736
Au	8.653967	4.262913	9.472784
Au	9.104179	2.842502	7.132699
Au	4.195695	2.852332	9.345503
Au	3.701888	5.948067	8.141227
Au	7.051136	1.290818	6.194288
Au	4.773202	0.793766	7.646925
Au	6.935307	2.128844	8.885339
Au	10.954423	4.757388	8.038953
Au	8.030363	6.325084	11.215684
Au	2.273182	3.245820	4.183381
Au	3.015937	5.169672	2.259037
Au	0.793766	5.634676	3.796160
Au	5.403348	6.289960	3.667996
Au	6.753979	3.996364	4.982488
Au	8.206646	6.142547	3.865531
Au	4.418499	1.639044	5.032856
Au	5.603675	5.173697	1.040304
Au	7.480574	3.356331	2.079397
Au	10.047313	4.280137	2.638663
Au	9.007763	2.340474	4.380108
Au	4.738828	3.089520	2.696866
Au	6.632264	1.158615	3.462748
Au	8.343076	5.763681	0.998591
Au	10.629862	4.419210	5.349775
Au	2.442511	7.809893	3.293626
Au	2.911988	9.887947	5.125049
Au	6.937603	8.169216	5.361807
Au	3.962411	7.455885	1.023246
Au	11.028426	6.661408	3.739161
Au	6.626488	7.910981	1.417994

Au	7.468043	9.939510	3.164110
Au	5.576314	10.822236	5.113710
Au	9.320089	8.138675	2.079896
Au	4.744027	9.321003	2.980295
Au	9.795349	8.966877	4.690943
Au	2.621795	2.449401	6.962848
Au	3.510946	5.089611	10.896404
Au	1.206034	4.777485	6.356107
Au	1.700321	4.074520	9.030757
Au	0.943422	6.690328	8.376388
Au	2.443680	9.010100	7.810358
Au	2.756719	7.692940	10.248780
Au	1.206023	7.597439	5.750725
Au	4.163841	7.508004	5.831929
Au	9.124460	9.093499	7.431892
Au	6.124460	7.373185	7.892811
Au	6.699114	10.408703	7.748480
Au	5.446500	7.094716	10.799370
Au	9.633347	6.960852	9.079049
Au	8.293313	11.061502	5.600385
Au	4.766128	9.457932	9.474347
Au	10.868078	7.109249	6.504411
Au	4.058754	11.168488	7.374994
Au	7.581641	8.747661	9.827044

Au_{58} structure 3: The DG structure (Dong and Gong, *J. Chem. Phys.*, 2010, **132**, 104301): forces converged to 0.03 eV/angstrom

Au	6.277991	9.777575	2.098340
Au	5.764889	8.767036	5.208198
Au	7.687457	7.386483	3.637236
Au	7.261040	4.784343	4.565157
Au	4.583651	4.393042	5.395484
Au	5.025793	6.510667	3.630352
Au	3.310764	10.578338	5.495975
Au	3.639785	9.552525	2.941761
Au	7.793572	10.738111	4.386878
Au	9.056052	9.387504	2.251188
Au	10.106367	4.467375	3.878785
Au	7.516652	3.038907	2.372510
Au	7.364212	7.596589	0.793766
Au	3.222615	5.267099	1.736298
Au	1.916675	7.677289	1.982792
Au	1.658124	3.889396	5.918558
Au	1.337926	5.851591	3.957779
Au	9.944061	9.066092	4.933004
Au	0.927397	6.537175	6.630114
Au	6.258936	1.787022	4.585561
Au	3.486915	1.823110	5.027273
Au	10.495650	7.082855	3.036862

Au	8.974251	2.121183	4.621403
Au	5.978458	5.154458	1.193312
Au	2.020741	3.295058	3.232179
Au	1.596174	8.542394	4.644113
Au	8.740351	5.395142	1.660918
Au	4.748199	3.124871	2.701579
Au	4.595789	7.684428	1.071661
Au	3.537552	3.546407	10.300333
Au	4.194598	5.208017	8.039492
Au	3.637391	7.099916	5.989848
Au	5.728422	7.546352	7.828917
Au	8.089287	7.248009	6.377085
Au	6.835341	4.907372	7.279004
Au	5.252158	0.793766	6.945033
Au	5.813134	2.549496	9.016604
Au	1.511428	4.565545	8.606634
Au	3.744515	11.120019	8.154058
Au	6.231472	10.087320	8.988757
Au	3.692952	6.285232	10.676190
Au	8.454931	6.129890	10.785712
Au	8.420195	3.754022	9.258876
Au	9.681720	3.966367	6.644147
Au	8.377131	10.195366	7.075888
Au	3.193135	2.438306	7.755033
Au	1.494479	7.212400	9.305981
Au	6.123618	7.701140	10.645674
Au	9.886580	6.034841	8.444265
Au	7.730706	2.040478	7.084919
Au	3.745307	8.838321	9.637665
Au	8.435207	8.430221	9.256946
Au	6.070239	4.842756	10.524982
Au	1.946440	9.100664	7.385370
Au	10.606300	8.562533	7.553874
Au	10.781790	6.399531	5.761380
Au	5.237867	11.646440	3.836065
Au	5.946744	11.360064	6.509225