

Supplementary information

Transport properties of a three-shell icosahedral matryoshka cluster: A first-principles study

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The calculated transmission spectra through the Pb@Mn₁₂@Pb₂₀ cluster connected to Au and Li electrodes with different anchoring configurations.

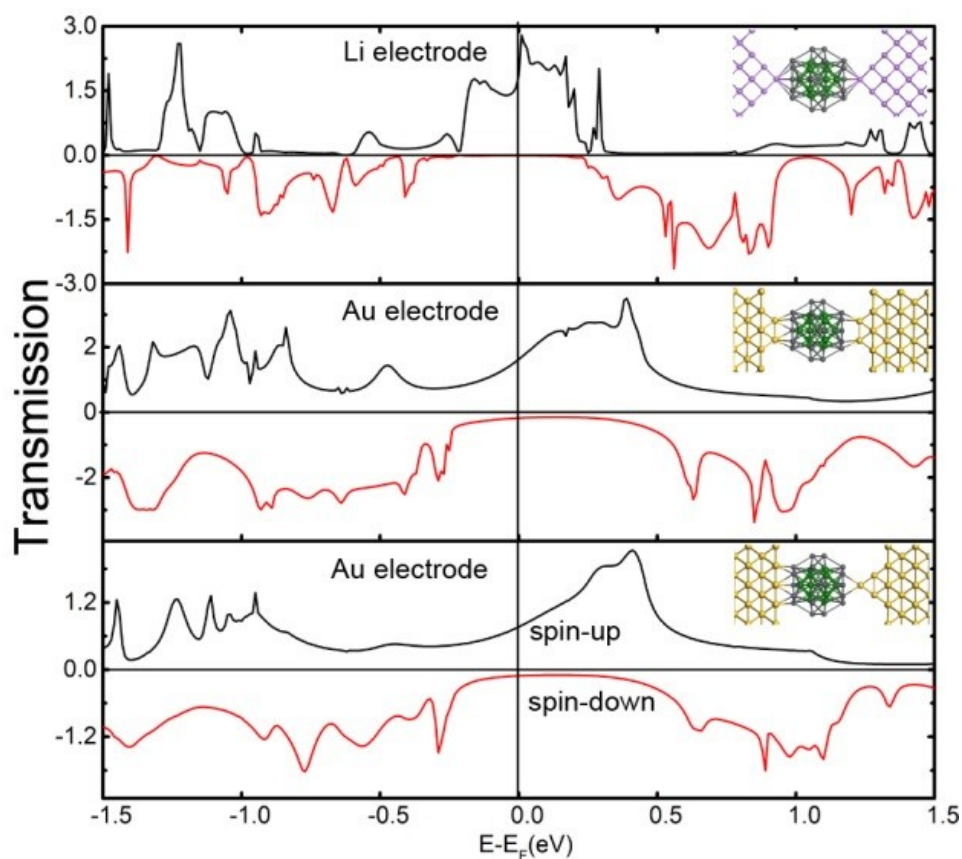


Figure S1 - Zero-bias energy dependent spin-resolved transmission spectra. Here, inserts schematically illustrate the examined junction.

Table S1-The coordinates of the Pb@Mn₁₂@Pb₂₀ cluster

Pb1	-2.791	0.000	-3.653
Pb2	-4.516	0.000	-0.862
Pb3	-3.653	-2.654	0.862
Pb4	-1.395	-4.295	-0.862
Pb5	-0.862	-2.654	-3.653
Pb6	1.395	-4.295	0.862
Pb7	2.258	-1.640	-3.653
Pb8	-0.862	2.654	-3.653
Pb9	-3.653	2.654	0.862
Pb10	-2.258	-1.640	3.653
Pb11	-2.258	1.640	3.653
Pb12	0.862	-2.654	3.653
Pb13	3.653	-2.654	-0.862
Pb14	2.258	1.640	-3.653
Pb15	-1.395	4.295	-0.862
Pb16	1.395	4.295	0.862
Pb17	0.862	2.654	3.653
Pb18	2.791	0.000	3.653
Pb19	4.516	0.000	0.862
Pb20	3.653	2.654	-0.862
Pb21	0.000	0.000	0.000
Mn22	-1.892	-1.374	-1.169
Mn23	-1.892	1.374	-1.169
Mn24	-2.338	0.000	1.169
Mn25	-0.723	-2.224	1.169
Mn26	0.723	-2.224	-1.169
Mn27	0.000	0.000	-2.614
Mn28	2.338	0.000	-1.169
Mn29	0.723	2.224	-1.169
Mn30	-0.723	2.224	1.169
Mn31	0.000	0.000	2.614
Mn32	1.892	-1.374	1.169
Mn33	1.892	1.374	1.169

Table S2 – The coordinates of Pb@Mn₁₂@Pb₂₀ cluster adsorption on Au(100) surface at the bridge site.

Pb1	8.850	6.393	4.689
Pb2	9.864	4.998	7.480
Pb3	11.504	7.256	9.205
Pb4	11.504	10.047	7.480
Pb5	9.864	9.514	4.689
Pb6	9.864	12.305	9.205
Pb7	7.209	11.442	4.689
Pb8	5.569	6.393	4.689
Pb9	7.209	4.135	9.205
Pb10	9.864	7.789	11.996
Pb11	7.209	5.860	11.996
Pb12	8.850	10.909	11.996
Pb13	7.209	13.167	7.480
Pb14	4.555	9.514	4.689
Pb15	4.555	4.998	7.480
Pb16	2.915	7.256	9.205
Pb17	4.555	7.789	11.996
Pb18	5.569	10.909	11.996
Pb19	4.555	12.305	9.205
Pb20	2.915	10.047	7.480
Pb21	7.209	8.651	8.343
Mn22	9.433	7.929	7.173
Mn23	7.209	6.313	7.173
Mn24	8.584	6.760	9.512
Mn25	9.433	9.374	9.512
Mn26	8.584	10.543	7.173
Mn27	7.209	8.651	5.728
Mn28	5.835	10.543	7.173
Mn29	4.986	7.929	7.173
Mn30	5.835	6.760	9.512
Mn31	7.209	8.651	10.957
Mn32	7.209	10.990	9.512
Mn33	4.986	9.374	9.512
Au1	0.000	0.000	0.000
Au2	1.442	1.442	2.039
Au3	2.884	0.000	0.000
Au4	4.326	1.442	2.039
Au5	5.768	0.000	0.000
Au6	7.209	1.442	2.039
Au7	8.651	0.000	0.000
Au8	10.093	1.442	2.039
Au9	11.535	0.000	0.000

Au10	12.977	1.442	2.039
Au11	14.419	0.000	0.000
Au12	15.861	1.442	2.039
Au13	0.000	2.884	0.000
Au14	1.442	4.326	2.039
Au15	2.884	2.884	0.000
Au16	4.326	4.326	2.039
Au17	5.768	2.884	0.000
Au18	7.209	4.326	2.039
Au19	8.651	2.884	0.000
Au20	10.093	4.326	2.039
Au21	11.535	2.884	0.000
Au22	12.977	4.326	2.039
Au23	14.419	2.884	0.000
Au24	15.861	4.326	2.039
Au25	0.000	5.768	0.000
Au26	1.442	7.209	2.039
Au27	2.884	5.768	0.000
Au28	4.326	7.209	2.039
Au29	5.768	5.768	0.000
Au30	7.209	7.209	2.039
Au31	8.651	5.768	0.000
Au32	10.093	7.209	2.039
Au33	11.535	5.768	0.000
Au34	12.977	7.209	2.039
Au35	14.419	5.768	0.000
Au36	15.861	7.209	2.039
Au37	0.000	8.651	0.000
Au38	1.442	10.093	2.039
Au39	2.884	8.651	0.000
Au40	4.326	10.093	2.039
Au41	5.768	8.651	0.000
Au42	7.209	10.093	2.039
Au43	8.651	8.651	0.000
Au44	10.093	10.093	2.039
Au45	11.535	8.651	0.000
Au46	12.977	10.093	2.039
Au47	14.419	8.651	0.000
Au48	15.861	10.093	2.039
Au49	0.000	11.535	0.000
Au50	1.442	12.977	2.039
Au51	2.884	11.535	0.000
Au52	4.326	12.977	2.039
Au53	5.768	11.535	0.000

Au54	7.209	12.977	2.039
Au55	8.651	11.535	0.000
Au56	10.093	12.977	2.039
Au57	11.535	11.535	0.000
Au58	12.977	12.977	2.039
Au59	14.419	11.535	0.000
Au60	15.861	12.977	2.039
Au61	0.000	14.419	0.000
Au62	1.442	15.861	2.039
Au63	2.884	14.419	0.000
Au64	4.326	15.861	2.039
Au65	5.768	14.419	0.000
Au66	7.209	15.861	2.039
Au67	8.651	14.419	0.000
Au68	10.093	15.861	2.039
Au69	11.535	14.419	0.000
Au70	12.977	15.861	2.039
Au71	14.419	14.419	0.000
Au72	15.861	15.861	2.039

Table S3 – The coordinates of atoms in the scattering region of Pb@Mn₁₂@Pb₂₀ junction, in which the cluster is sandwiched between two Au (100) electrodes

Au	2.163	2.163	1.249
Au	5.047	2.163	1.249
Au	7.930	2.163	1.249
Au	10.814	2.163	1.249
Au	13.698	2.163	1.249
Au	2.163	5.047	1.249
Au	5.047	5.047	1.249
Au	7.930	5.047	1.249
Au	10.814	5.047	1.249
Au	13.698	5.047	1.249
Au	2.163	7.930	1.249
Au	5.047	7.930	1.249
Au	7.930	7.930	1.249
Au	10.814	7.930	1.249
Au	13.698	7.930	1.249
Au	2.163	10.814	1.249
Au	5.047	10.814	1.249
Au	7.930	10.814	1.249
Au	10.814	10.814	1.249
Au	13.698	10.814	1.249
Au	2.163	13.698	1.249

Au	5.047	13.698	1.249
Au	7.930	13.698	1.249
Au	10.814	13.698	1.249
Au	13.698	13.698	1.249
Au	0.721	0.721	3.288
Au	3.605	0.721	3.288
Au	6.488	0.721	3.288
Au	9.372	0.721	3.288
Au	12.256	0.721	3.288
Au	0.721	3.605	3.288
Au	3.605	3.605	3.288
Au	6.488	3.605	3.288
Au	9.372	3.605	3.288
Au	12.256	3.605	3.288
Au	0.721	6.488	3.288
Au	3.605	6.488	3.288
Au	6.488	6.488	3.288
Au	9.372	6.488	3.288
Au	12.256	6.488	3.288
Au	0.721	9.372	3.288
Au	3.605	9.372	3.288
Au	6.488	9.372	3.288
Au	9.372	9.372	3.288
Au	12.256	9.372	3.288
Au	0.721	12.256	3.288
Au	3.605	12.256	3.288
Au	6.488	12.256	3.288
Au	9.372	12.256	3.288
Au	12.256	12.256	3.288
Pb	6.274	4.208	5.938
Pb	9.587	4.208	5.938
Pb	5.250	7.359	5.938
Pb	10.611	7.359	5.938
Pb	7.930	9.307	5.938
Mn	7.930	6.488	6.979
Mn	7.930	4.119	8.443
Mn	5.677	5.756	8.443
Mn	10.184	5.756	8.443
Mn	6.538	8.405	8.443
Mn	9.323	8.405	8.443
Pb	5.250	2.799	8.757
Pb	10.611	2.799	8.757
Pb	3.593	7.898	8.757
Pb	12.268	7.898	8.757

Pb	7.930	11.049	8.757
Pb	7.930	6.488	9.628
Pb	7.930	1.928	10.499
Pb	3.593	5.079	10.499
Pb	12.268	5.079	10.499
Pb	5.250	10.178	10.499
Pb	10.611	10.178	10.499
Mn	6.538	4.572	10.812
Mn	9.323	4.572	10.812
Mn	5.677	7.221	10.812
Mn	10.184	7.221	10.812
Mn	7.930	8.858	10.812
Mn	7.930	6.488	12.277
Pb	7.930	3.670	13.317
Pb	5.250	5.618	13.317
Pb	10.611	5.618	13.317
Pb	6.274	8.769	13.317
Pb	9.587	8.769	13.317
Au	7.930	5.047	15.967
Au	7.930	7.930	15.967
Au	0.721	0.721	18.006
Au	3.605	0.721	18.006
Au	6.488	0.721	18.006
Au	9.372	0.721	18.006
Au	12.256	0.721	18.006
Au	0.721	3.605	18.006
Au	3.605	3.605	18.006
Au	6.488	3.605	18.006
Au	9.372	3.605	18.006
Au	12.256	3.605	18.006
Au	0.721	6.488	18.006
Au	3.605	6.488	18.006
Au	6.488	6.488	18.006
Au	9.372	6.488	18.006
Au	12.256	6.488	18.006
Au	0.721	9.372	18.006
Au	3.605	9.372	18.006
Au	6.488	9.372	18.006
Au	9.372	9.372	18.006
Au	12.256	9.372	18.006
Au	0.721	12.256	18.006
Au	3.605	12.256	18.006
Au	6.488	12.256	18.006
Au	9.372	12.256	18.006

Au	12.256	12.256	18.006
Au	2.163	2.163	20.045
Au	5.047	2.163	20.045
Au	7.930	2.163	20.045
Au	10.814	2.163	20.045
Au	13.698	2.163	20.045
Au	2.163	5.047	20.045
Au	5.047	5.047	20.045
Au	7.930	5.047	20.045
Au	10.814	5.047	20.045
Au	13.698	5.047	20.045
Au	2.163	7.930	20.045
Au	5.047	7.930	20.045
Au	7.930	7.930	20.045
Au	10.814	7.930	20.045
Au	13.698	7.930	20.045
Au	2.163	10.814	20.045
Au	5.047	10.814	20.045
Au	7.930	10.814	20.045
Au	10.814	10.814	20.045
Au	13.698	10.814	20.045
Au	2.163	13.698	20.045
Au	5.047	13.698	20.045
Au	7.930	13.698	20.045
Au	10.814	13.698	20.045
Au	13.698	13.698	20.045
Au	0.721	0.721	22.085
Au	3.605	0.721	22.085
Au	6.488	0.721	22.085
Au	9.372	0.721	22.085
Au	12.256	0.721	22.085
Au	0.721	3.605	22.085
Au	3.605	3.605	22.085
Au	6.488	3.605	22.085
Au	9.372	3.605	22.085
Au	12.256	3.605	22.085
Au	0.721	6.488	22.085
Au	3.605	6.488	22.085
Au	6.488	6.488	22.085
Au	9.372	6.488	22.085
Au	12.256	6.488	22.085
Au	0.721	9.372	22.085
Au	3.605	9.372	22.085
Au	6.488	9.372	22.085

Au	9.372	9.372	22.085
Au	12.256	9.372	22.085
Au	0.721	12.256	22.085
Au	3.605	12.256	22.085
Au	6.488	12.256	22.085
Au	9.372	12.256	22.085
Au	12.256	12.256	22.085