

SUPPORTING INFORMATION

Structural and electronic features of small hybrid organic-inorganic halide perovskite clusters: a theoretical analysis

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Optimized structure of **1d** cluster (b3lyp/6-311G++)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
53	6.592403	6.194952	6.854310
7	9.035683	5.166632	4.495069
7	5.619745	8.679173	9.193401
1	6.499804	8.689417	9.740994
1	8.202934	5.228233	5.109020
1	5.666942	9.496104	8.557763
1	5.668020	7.839360	8.587677
1	9.044680	6.038376	3.934427
1	9.859919	5.218882	5.121150
53	11.456231	6.174235	6.887257
6	9.034870	3.936300	3.643974
7	12.422527	8.648260	9.240452
1	12.375974	7.807760	8.635689
1	9.929094	3.929843	3.027990
1	12.389113	9.464310	8.602721
1	11.535668	8.665892	9.776802
1	9.022821	3.060312	4.285545
1	8.152055	3.942342	3.011737
53	6.619400	11.054709	6.750955
6	4.402088	8.693154	10.062392
7	9.068003	11.969175	4.348773
1	3.516718	8.679546	9.433891
1	8.236091	11.940700	4.966271
1	4.409236	9.593148	10.669883
1	4.412862	7.816355	10.702810
1	9.892941	11.935611	4.975056
1	9.067937	11.074577	3.825127
82	9.036702	8.617461	6.819469
53	11.474698	11.031333	6.784715
53	9.060220	8.545270	3.383657
53	9.013937	8.692362	10.257063
6	9.076226	13.163096	3.447375
6	13.629390	8.655997	10.124443
1	13.621091	9.557726	10.729327
1	9.967608	13.134540	2.827912
1	14.522349	8.634471	9.506983
1	13.604558	7.781113	10.767111
1	8.190534	13.140368	2.819598
1	9.076326	14.065019	4.052071

Optimized structure of 2e cluster (b3lyp/6-311G++)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
6	4.336457	6.326819	2.897790
7	3.972125	4.937641	2.466838
53	0.490566	4.466080	3.148164
7	0.700884	3.072345	-1.069406
6	-0.393784	4.071850	-1.311517
53	-0.084896	-1.979988	4.587225
82	0.234119	1.302403	3.398180
53	2.555235	0.613639	1.456539
53	1.198769	-4.170414	-0.161891
7	2.833439	-1.923841	-2.412358
6	3.085442	-2.873977	-3.545720
53	1.437352	1.016369	-3.923237
7	-1.545363	-2.554563	1.385386
6	-2.830090	-3.316540	1.278550
53	-1.872296	1.055428	1.137956
1	-2.664200	-4.334256	1.617428
1	-3.580051	-2.836101	1.899576
1	-3.154561	-3.323747	0.242343
1	2.131759	-3.187973	-3.957202
1	3.670937	-2.366030	-4.305281
1	3.626547	-3.735394	-3.167835
1	3.695313	7.031990	2.378356
1	4.195089	6.413356	3.970502
1	5.375011	6.512944	2.643155
1	-0.469879	4.720543	-0.444362
1	-0.141007	4.651374	-2.193671
1	-1.327871	3.540333	-1.461174
1	0.824286	2.439812	-1.885199
1	1.606172	3.556393	-0.921679
1	0.498488	2.489850	-0.253404
1	4.597281	4.239880	2.900274
1	4.037351	4.848212	1.434020
1	2.993307	4.715814	2.726482
1	3.727045	-1.577935	-2.024694
1	2.300925	-1.096418	-2.743117
1	2.302545	-2.399517	-1.660692
1	-1.656874	-1.573235	1.085320
1	-1.201909	-2.517458	2.366015
1	-0.791122	-2.995572	0.819110
82	6.500526	0.534516	1.369773
53	6.306270	-1.996124	3.251067
53	6.126914	-0.557881	-1.746542
53	3.811130	4.936217	-1.078670
53	6.430169	2.750559	3.978358
53	9.584145	0.539652	1.381455
7	2.825007	-3.206058	2.879273
6	3.126366	-4.521717	3.535163
1	3.448427	-4.341163	4.555600
1	2.224203	-5.124950	3.528549
1	3.912635	-5.020867	2.978406
1	3.661725	-2.609443	2.855385
1	2.482491	-3.359293	1.911040
1	2.071767	-2.710919	3.392782
7	4.695048	2.359851	-3.345459
1	3.756309	1.996149	-3.609683
6	5.445759	2.865239	-4.538034
1	5.197109	1.586993	-2.875134
1	4.539885	3.116808	-2.650331
1	6.418605	3.226832	-4.218869
1	5.567681	2.055545	-5.251218
1	4.882181	3.675431	-4.990336
7	8.756417	0.205426	4.809636
1	8.153228	-0.626050	4.725133
6	9.721527	0.117520	5.951201
1	8.123859	1.024484	4.879158
1	9.236914	0.303527	3.891009
1	10.314561	1.026475	5.980700
1	9.170178	0.007357	6.880027
1	10.371692	-0.739629	5.802056

Optimized structure of **8c** cluster (PM6)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	-0.196169	-0.112638	-0.170154
53	2.957308	0.045000	-0.024536
53	0.127183	2.881854	0.153581
53	-0.036394	0.104632	2.857119
53	-3.037132	0.033555	-0.027607
53	0.245957	-3.010361	0.099832
53	0.284687	0.286463	-3.073841
82	-0.239519	-0.204203	5.936310
53	2.785481	0.024293	5.611517
53	-0.067387	2.820771	5.739218
53	-0.052432	0.008131	8.805724
53	-3.152159	-0.021300	5.685175
53	0.138521	-3.095064	5.454421
82	-0.072831	5.900518	-0.065212
53	2.936845	5.822824	0.096882
53	-0.065977	8.793734	-0.009742
53	0.065984	5.705428	2.893856
53	-3.026916	5.518851	0.231857
53	0.273166	5.543830	-3.045071
82	-0.232450	5.877414	5.958332
53	2.798272	5.582343	5.650560
53	0.131685	8.735821	5.587912
53	0.087568	5.601697	8.825525
53	-3.119043	5.558145	5.500068
82	5.859395	-0.092871	-0.129250
53	8.988062	-0.424842	-0.034868
53	5.926719	2.818088	-0.101884
53	5.720140	-0.121768	2.773444
53	5.714231	-3.198492	-0.115328
53	5.849656	-0.269386	-3.226136
82	5.765185	-0.158145	5.792973
53	8.734144	0.246400	5.483038
53	5.518835	2.824239	5.546536
53	5.463995	0.153186	8.721388
53	5.717230	-3.073843	5.749710
82	5.913195	6.064578	-0.186987
53	8.877530	5.796258	0.022893
53	5.824273	8.928343	0.068464
53	5.744137	5.763382	2.810242
53	5.627497	5.738418	-3.087456
82	5.844600	5.861983	5.843904
53	8.735300	5.512038	5.549691
53	5.472631	8.742078	5.662195
53	5.419614	5.452222	8.752442
6	-3.057224	-3.239275	1.994290
7	-2.440864	-2.387461	3.061931
1	-3.141693	-2.023508	3.744609
1	-1.701095	-2.908697	3.609240
1	-1.959273	-1.544432	2.630104
1	-3.556965	-4.126401	2.408757
1	-2.273450	-3.577153	1.267448
1	-3.786211	-2.659143	1.390048
6	-3.048297	2.148391	-3.178246
7	-2.290924	3.170701	-2.386773
1	-1.727691	3.814593	-2.998226
1	-2.919972	3.761601	-1.788596
1	-1.602375	2.697861	-1.730170
1	-3.776129	2.609390	-3.860769
1	-3.584700	1.442996	-2.499169
1	-2.350301	1.512117	-3.769692
6	-3.724965	2.431727	2.827546
7	-2.337396	2.997757	2.881232
1	-1.620382	2.225584	2.939963
1	-2.130308	3.567156	2.019152
1	-2.217970	3.621219	3.721629
1	-3.844210	1.769780	1.937268
1	-4.482670	3.230977	2.768191
1	-3.933505	1.812793	3.730134
6	-3.241107	3.669705	8.880630
7	-2.536495	2.576737	8.136328
1	-3.196952	1.945357	7.626192

1	-1.882181	2.993803	7.404462
1	-1.943619	1.979495	8.763338
1	-3.810199	4.321900	8.178313
1	-2.502845	4.348192	9.373645
1	-3.929552	3.278841	9.643289
6	-2.947646	9.399643	2.770191
7	-2.473867	7.983664	2.905846
1	-2.731272	7.404445	2.059799
1	-1.421780	7.951290	2.993683
1	-2.865643	7.510145	3.766184
1	-2.515150	9.868311	1.859298
1	-2.630276	10.006054	3.641662
1	-4.046355	9.454595	2.692317
6	2.489164	-3.588187	-3.009220
7	2.776144	-2.209964	-2.495054
1	2.014618	-1.519233	-2.786873
1	2.792076	-2.204255	-1.435941
1	3.703889	-1.841555	-2.823391
1	1.516805	-3.952318	-2.601175
1	3.266578	-4.304436	-2.686481
1	2.420461	-3.606444	-4.109127
6	3.348975	-3.569160	2.860691
7	2.610942	-2.266740	2.798111
1	1.969844	-2.236716	1.958995
1	2.024228	-2.125386	3.661950
1	3.280301	-1.459477	2.726530
1	2.654800	-4.419785	2.950278
1	4.041246	-3.590795	3.738701
1	3.971311	-3.718322	1.949662
6	2.006235	-3.218762	8.813746
7	3.048148	-2.461875	8.047422
1	2.594218	-1.882654	7.280556
1	3.582267	-1.792052	8.654703
1	3.745467	-3.091995	7.579328
1	1.267855	-2.514944	9.272048
1	2.444272	-3.839024	9.608811
1	1.408841	-3.867762	8.135038
6	3.394224	2.693343	-3.517318
7	2.805220	3.019579	-2.178074
1	2.276723	2.196749	-1.788276
1	3.556652	3.275421	-1.489412
1	2.134472	3.832370	-2.248989
1	4.101765	1.835252	-3.443635
1	3.961451	3.560128	-3.919254
1	2.606937	2.419910	-4.241798
6	3.435346	2.895195	2.287471
7	2.346136	2.856916	3.308890
1	1.590420	3.544283	3.068010
1	1.917796	1.902216	3.360308
1	2.720947	3.105815	4.253883
1	3.053735	2.613224	1.285409
1	4.258256	2.200435	2.554919
1	3.872967	3.914958	2.209306
6	2.554002	2.673588	9.475315
7	2.830652	2.864326	8.013349
1	3.218772	1.986384	7.585576
1	1.948341	3.111109	7.492757
1	3.529549	3.640190	7.860233
1	1.820248	1.847490	9.630014
1	2.122503	3.593296	9.918519
1	3.478024	2.416663	10.025013
6	3.619503	8.997202	-3.107778
7	2.552845	8.206701	-2.413794
1	1.997043	7.612955	-3.077275
1	2.987780	7.540187	-1.705073
1	1.877137	8.812241	-1.884700
1	4.338028	8.316738	-3.625938
1	4.236057	9.563541	-2.372086
1	3.204133	9.701446	-3.842534
6	2.813125	9.320111	2.366793
7	2.874702	8.024493	3.116176
1	2.014745	7.888785	3.708479
1	2.940245	7.209434	2.451341
1	3.716651	7.994555	3.749249
1	1.917536	9.349221	1.698658
1	3.710014	9.443681	1.715283
1	2.759219	10.180140	3.052265

6	2.820710	9.356953	8.567434
7	2.824126	7.900900	8.209153
1	2.821198	7.780380	7.158047
1	3.685975	7.404436	8.567033
1	1.968057	7.401533	8.576024
1	3.713830	9.864464	8.144028
1	2.821558	9.508227	9.658972
1	1.923588	9.859272	8.146773
6	8.950980	-3.618667	-3.282604
7	8.132309	-2.695180	-2.437722
1	7.534085	-2.024161	-3.019506
1	7.447586	-3.216470	-1.792990
1	8.731498	-2.081409	-1.794390
1	8.310460	-4.238636	-3.936574
1	9.554011	-4.304436	-2.659389
1	9.648162	-3.058475	-3.932293
6	8.762912	-3.634311	3.412331
7	8.221988	-2.307551	2.970977
1	7.171534	-2.342998	2.872503
1	8.432641	-1.553018	3.694859
1	8.612202	-1.992420	2.044559
1	8.299928	-3.929678	4.385707
1	9.854757	-3.597221	3.564000
1	8.531538	-4.428379	2.681985
6	8.955899	2.240620	-2.985102
7	8.208931	3.465544	-2.556824
1	7.893859	4.054030	-3.355601
1	7.328618	3.184159	-2.009449
1	8.774528	4.077705	-1.902295
1	8.316378	1.588997	-3.618548
1	9.227871	1.618493	-2.095262
1	9.876879	2.485231	-3.533972
6	9.191892	2.712251	2.220911
7	7.949670	2.946549	3.025319
1	7.131703	3.158458	2.397826
1	7.707898	2.100972	3.601397
1	8.070647	3.764176	3.684156
1	9.067694	1.840725	1.536792
1	10.059193	2.512819	2.870514
1	9.420913	3.598397	1.584011
6	8.759830	3.648891	8.841893
7	7.961339	2.636538	8.077722
1	8.557390	2.079207	7.415375
1	7.460347	1.963433	8.705940
1	7.218786	3.117055	7.489583
1	9.533189	3.180121	9.466521
1	8.097928	4.269366	9.486906
1	9.249262	4.369342	8.140799
6	8.812616	8.941292	3.824014
7	8.223291	8.156263	2.691900
1	7.560299	8.730976	2.110883
1	8.947951	7.764412	2.053471
1	7.661336	7.331003	3.069027
1	9.398390	9.802680	3.474273
1	9.457098	8.296200	4.461360
1	8.003048	9.308982	4.505965

Optimized structure of **12b** cluster (PM6)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
82	-0.179538	-0.207482	-0.183058
53	2.861867	-0.017485	-0.009867
53	0.013418	2.814877	0.066323
53	0.021393	0.097990	2.800050
53	-3.071194	-0.043878	-0.008544
53	0.127145	-3.114488	0.184064
53	0.103861	0.183528	-3.101821
82	-0.141781	-0.180119	5.778946
53	2.906395	0.004863	5.506192
53	0.068755	2.810108	5.605486
53	0.285477	0.156485	8.720571
53	-2.997303	-0.052082	5.723964
53	0.210292	-3.107367	5.404514
82	-0.194012	5.826843	-0.145558
53	2.849149	5.509128	0.047004
53	0.173228	8.730811	0.217737
53	0.089976	5.676147	2.872397
53	-3.052041	5.549162	0.230933
53	0.157957	5.519765	-3.052337
82	-0.186359	5.841967	5.903839
53	2.870823	5.621236	5.605272
53	-0.064738	8.724415	5.722347
53	0.185692	5.371274	8.776502
53	-3.042511	5.442182	5.548620
82	5.751624	-0.231089	-0.223871
53	8.628550	-0.056816	-0.003151
53	5.727758	2.735593	-0.506671
53	5.797049	-0.563378	2.758944
53	5.776892	-3.297911	-0.430587
53	5.783807	-0.421192	-3.249226
82	5.776917	-0.201347	5.710517
53	8.649907	0.057684	5.648210
53	5.869542	2.800191	5.892080
53	5.617713	-0.249416	8.753374
53	5.824469	-3.212794	6.006710
82	5.734459	5.668542	-0.115666
53	8.599980	5.569380	0.114184
53	5.540078	8.681141	-0.104295
53	5.728640	5.802770	2.853315
53	5.740173	6.012733	-3.163706
82	5.753929	5.739262	5.776945
53	8.643870	5.642137	5.659167
53	5.738788	8.777516	6.028250
53	5.794362	5.927207	8.859665
82	11.624448	-0.125336	-0.130483
53	14.549781	0.219572	0.190042
53	11.389145	2.840429	0.161267
53	11.411457	0.069641	2.890501
53	11.379470	-3.085626	0.202943
53	11.363891	0.173158	-3.018535
82	11.655185	-0.171186	5.887629
53	14.548996	0.206985	5.564489
53	11.453423	2.869668	5.706481
53	11.331101	0.200313	8.799169
53	11.302131	-3.061449	5.625141
82	11.642651	5.850083	-0.101287
53	14.524206	5.645365	0.016139
53	11.239243	8.727922	0.231443
53	11.476639	5.621485	2.905845
53	11.249312	5.507576	-3.012960
82	11.685527	5.877501	5.943402
53	14.555856	5.651385	5.641854
53	11.297951	8.768965	5.533240
53	11.256661	5.575740	8.824988
6	-3.713179	-2.862396	2.939461
7	-2.260719	-2.506121	2.830599

1	-1.821887	-2.887634	1.949469
1	-2.137478	-1.456418	2.802623
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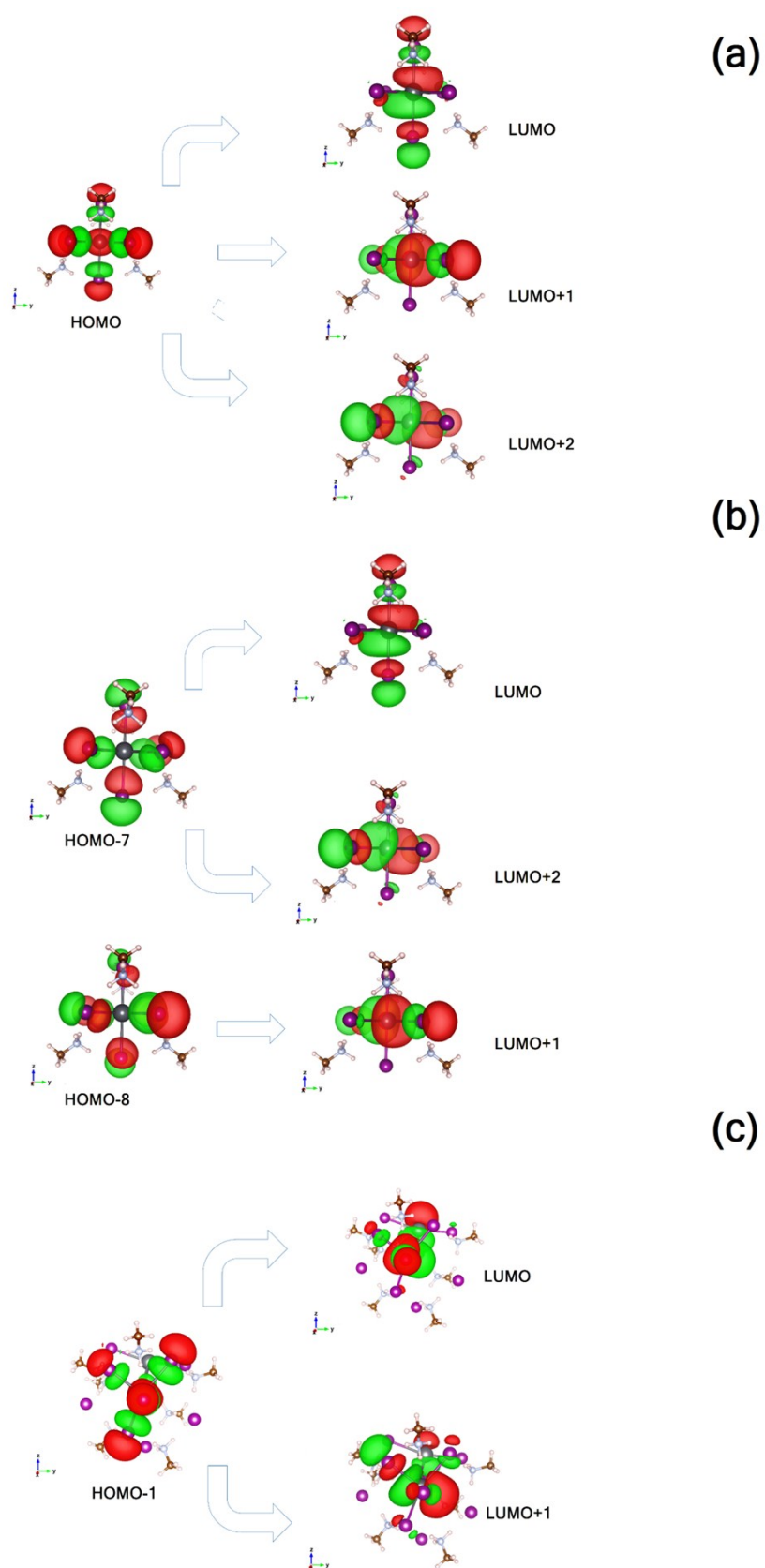


Figure 1 S.I.: Molecular orbitals involved in the main transitions in **1d** (a) at ~ 300 nm, (b) at ~ 260 nm, (c) **2e** at ~ 310 nm. (Isosurface value = 0.02).

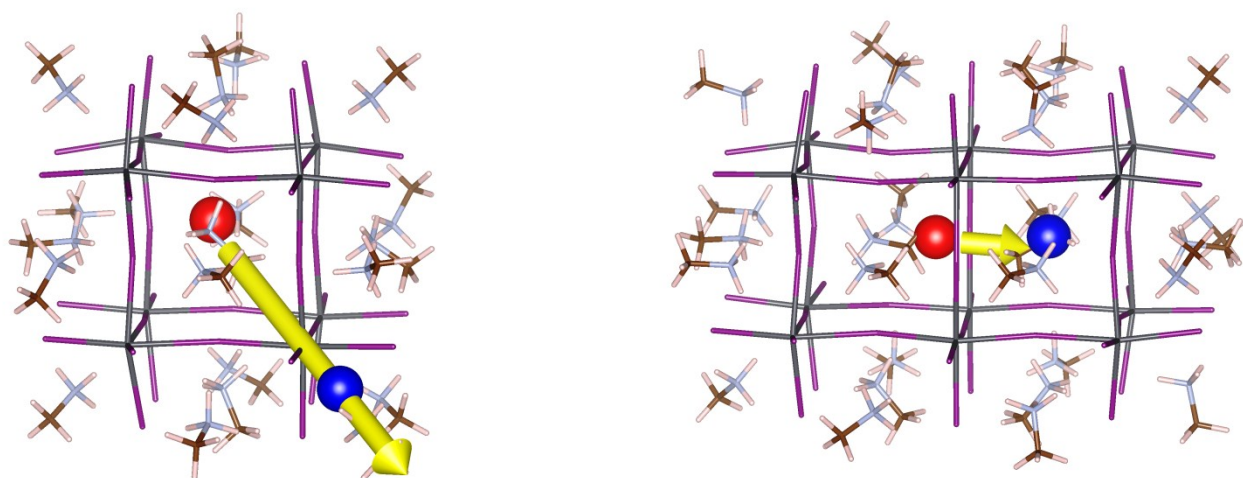


Fig 2 S.I.: (Left) 3D representation of the center of HOMO (red sphere), LUMO (blue sphere), and the intensity of the EDM (yellow arrow) for the most stable Pb octamer structure, i.e. **8c**. (Right) Same for the most stable Pb dodecamer structure (**12b**).