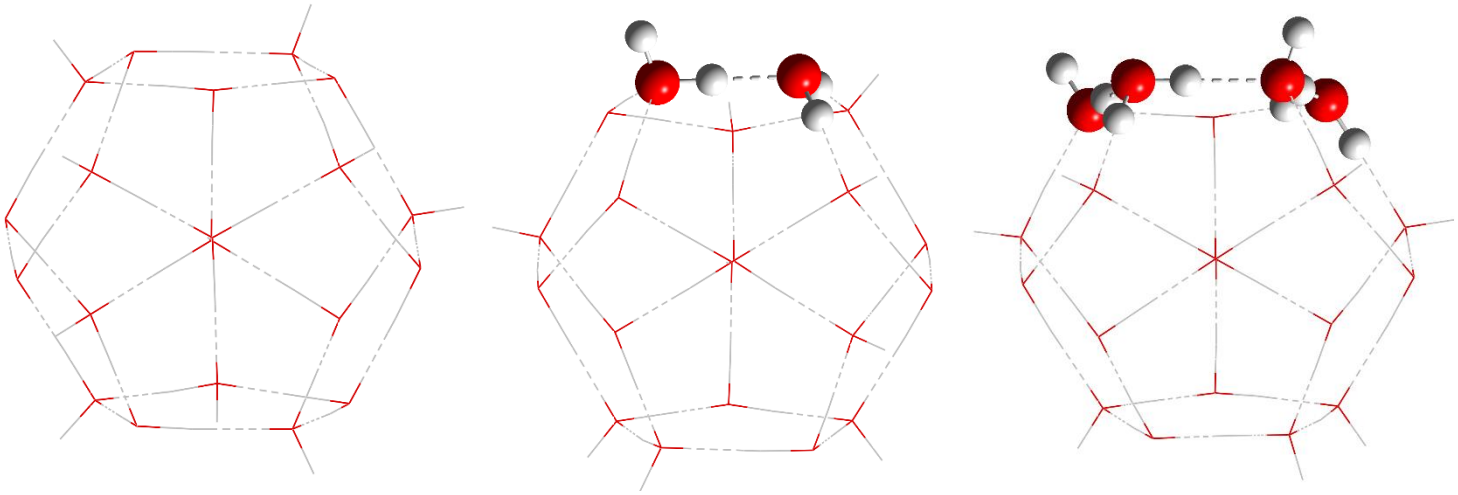
Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Supplementary Table 1. The stabilization energy (SE) and stabilization energy per water molecule (SEP) in kcal/mol, for the most stable isomers of fused cages obtained for different functional using cc-pVTZ basis set. The BSSE corrected energy values are given in parentheses.

System	B97-D/cc-pVTZ		M06-HF/cc-pVTZ		M06-2X/cc-pVTZ		M06/cc-pVTZ		M06-L/cc-pVTZ	
	SE	SEP	SE	SEP	SE	SEP	SE	SEP	SE	SEP
FDD	-452.28 (-357.76)	-12.92 (-10.22)	-447.72 (-378.70)	-12.79 (-10.82)	-437.16 (-368.13)	-12.49 (-10.52)	-411.76 (-342.73)	-11.76 (-9.79)	-407.15 (-350.67)	-11.63 (-10.02)
FDI	-446.98 (-353.04)	-12.77 (-10.08)	-442.14 (-366.84)	-12.63 (-10.48)	-433.08 (-364.05)	-12.37 (-10.40)	-410.86 (-335.56)	-11.73 (-9.58)	-404.43 (-341.68)	-11.55 (-9.76)
FII	-452.74 (-357.88)	-12.56 (-9.94)	-452.74 (-377.43)	-12.58 (-10.48)	-442.05 (-373.02)	-12.28 (-10.36)	-418.08 (-342.77)	-11.61 (-9.52)	-410.69 (-347.94)	-11.40 (-9.66)



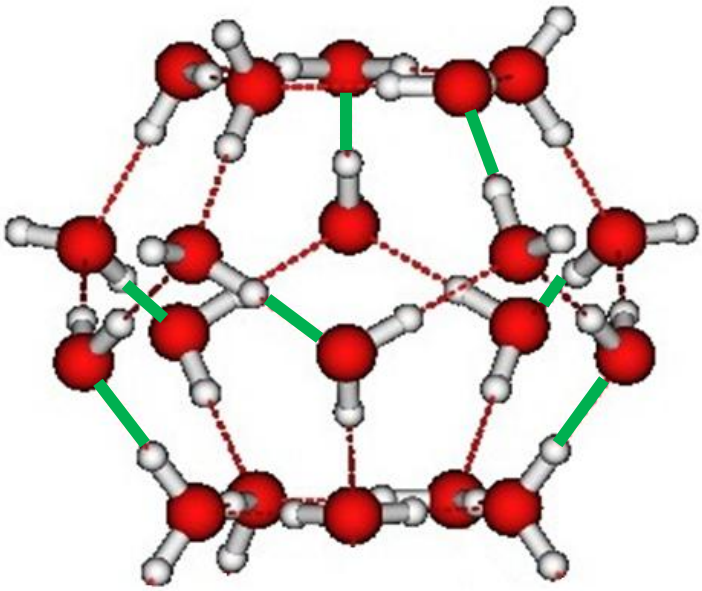
t*1d* = 0
(a)

t*1d* = 1
(b)

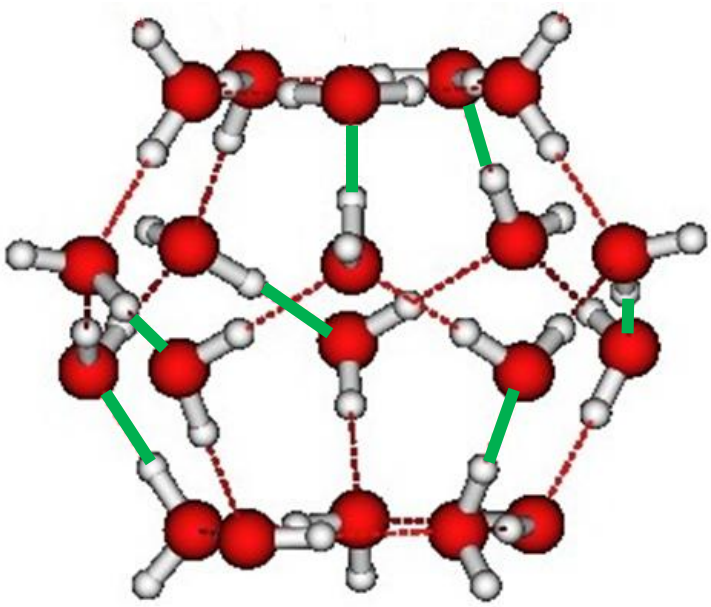
t*1d* = 2
(c)

Supplementary Figure 1. Three different types of five- membered rings present in the dodecahedral water cage each differ in the number of *t1d* hydrogen bonds. The *t1d* hydrogen bonds are shown using ball and stick model.

(a)



DD (7)



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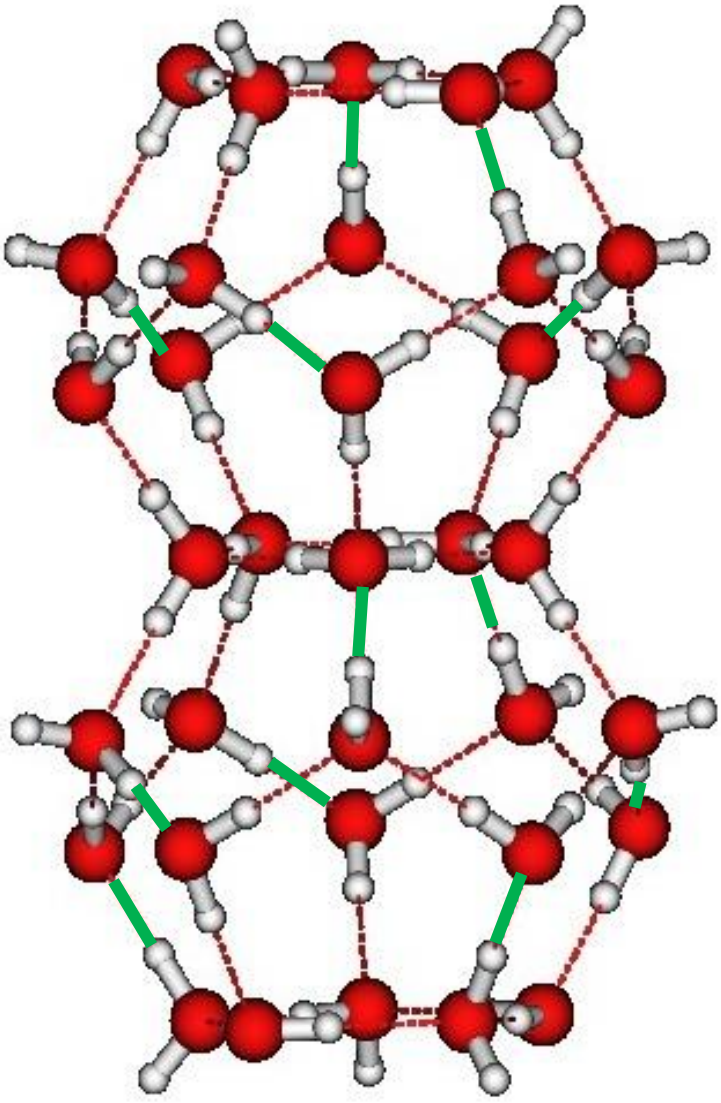
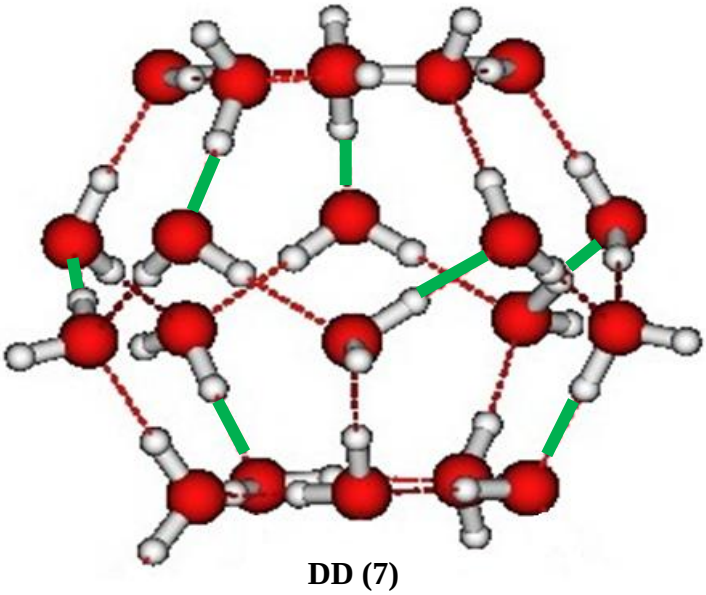


FDD (12)

(b)



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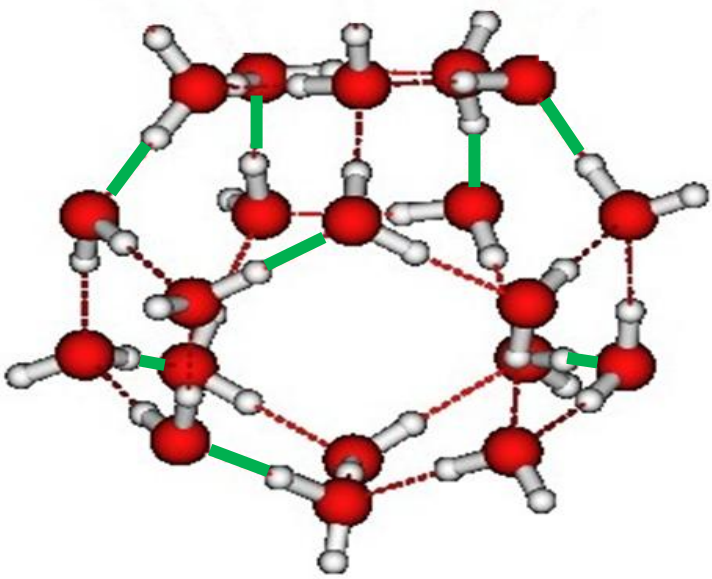
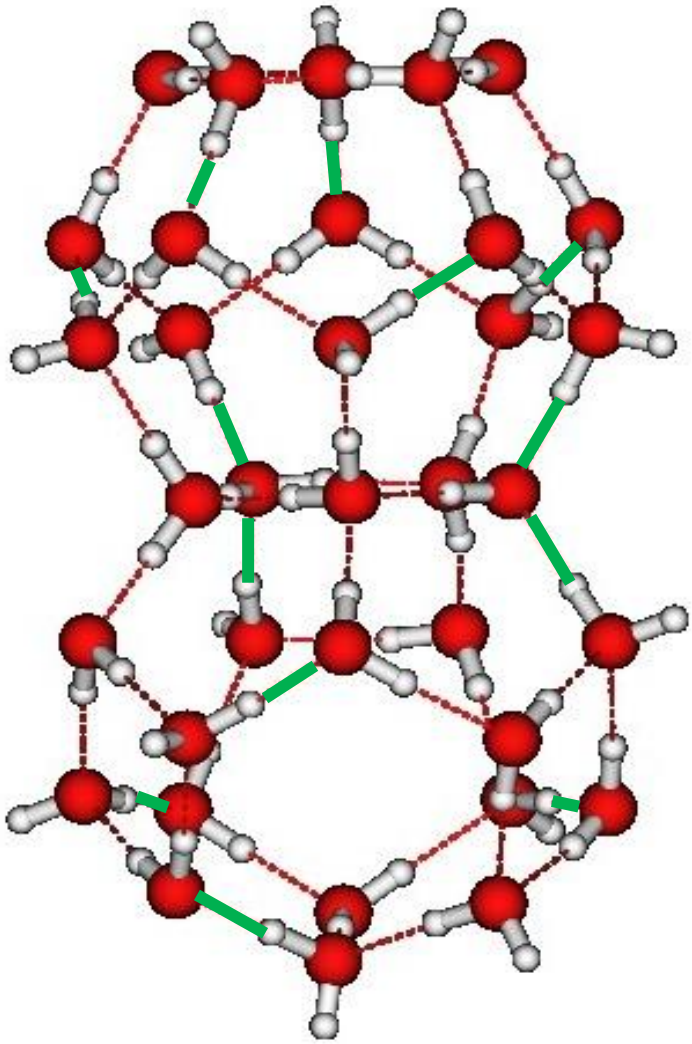
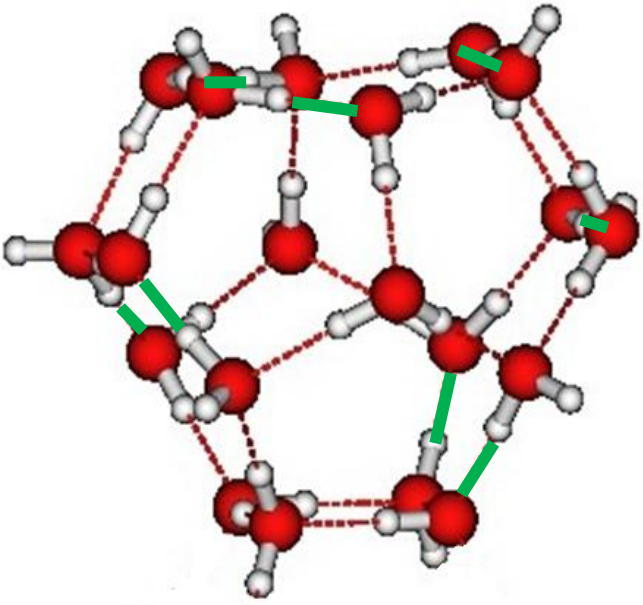


IDD (8)



FDI (13)

(c)



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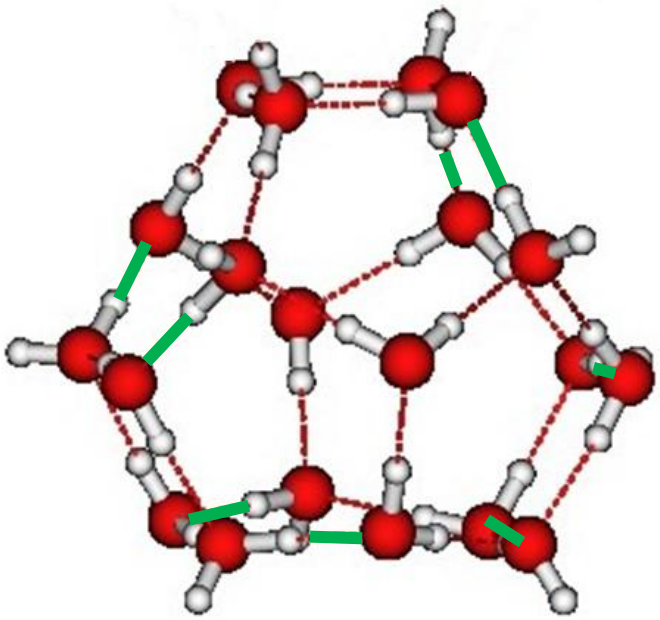
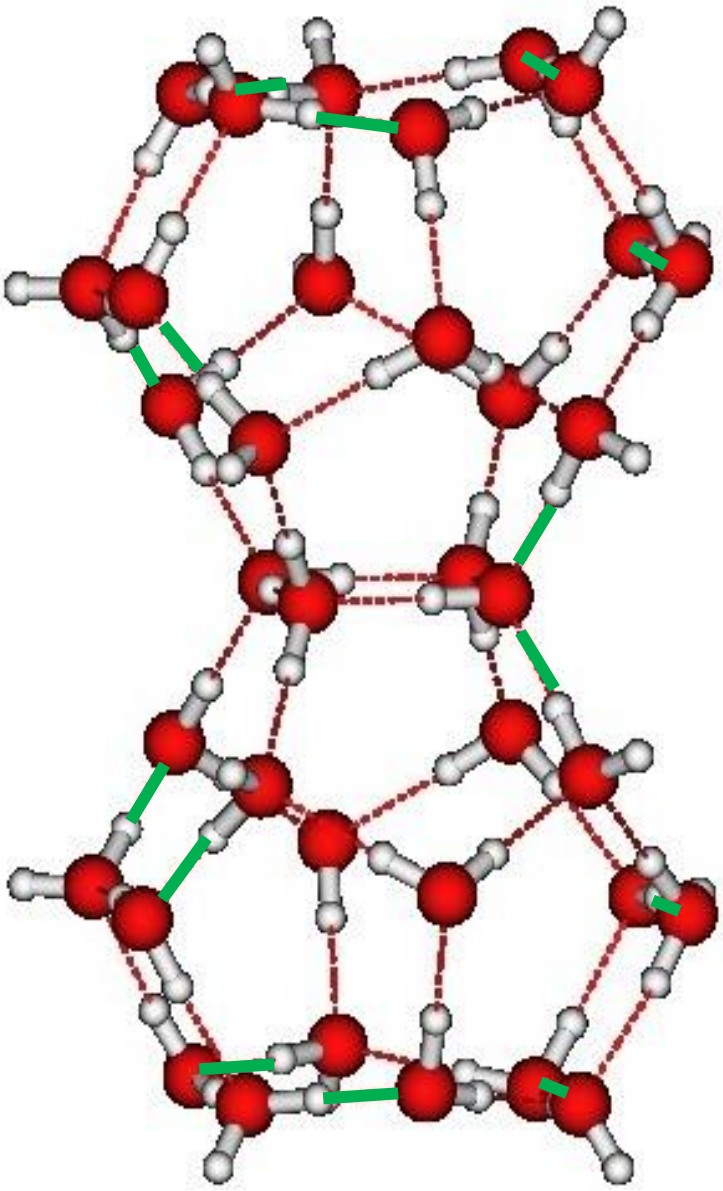
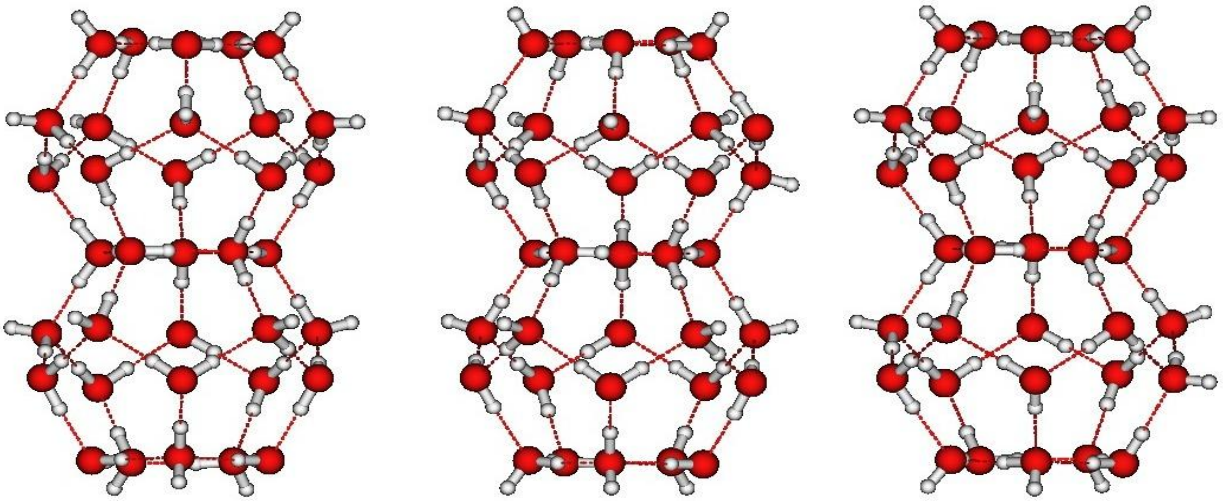


IDD (8)



FII (14)

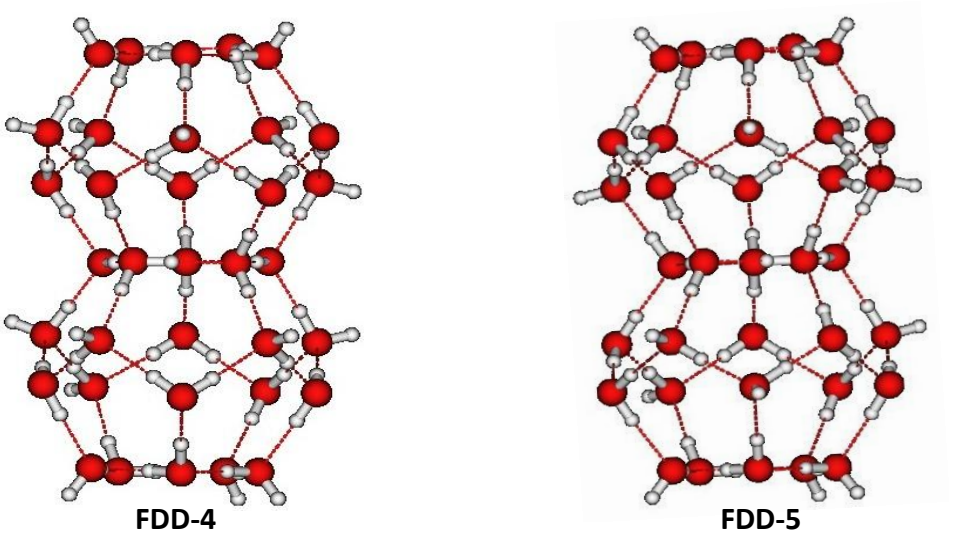
Supplementary figure 2. The optimized geometries of the single and the fused cages of dodecahedral and irregular dodecahedral water clusters. The number of *t1d* hydrogen bonds in each case is given in parenthesis.



FDD-1
(-452.28)
12

FDD-2
(-450.20)
12

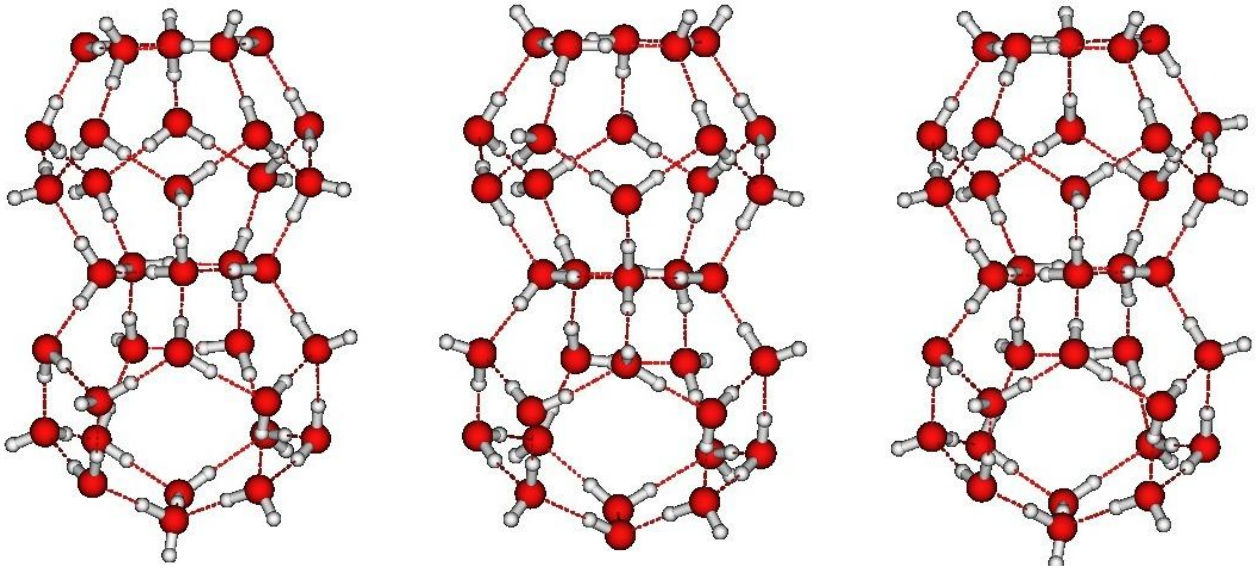
FDD-3
(-450.17)
11



FDD-4
(-448.08)
11

FDD-5
(-445.29)
10

Supplementary Figure 3. The optimized geometries of various fused dodecahedral cages (FDD). The stabilization energy without BSSE correction is given in parentheses. The number of t1d hydrogen bonds present in each case is given in italics.

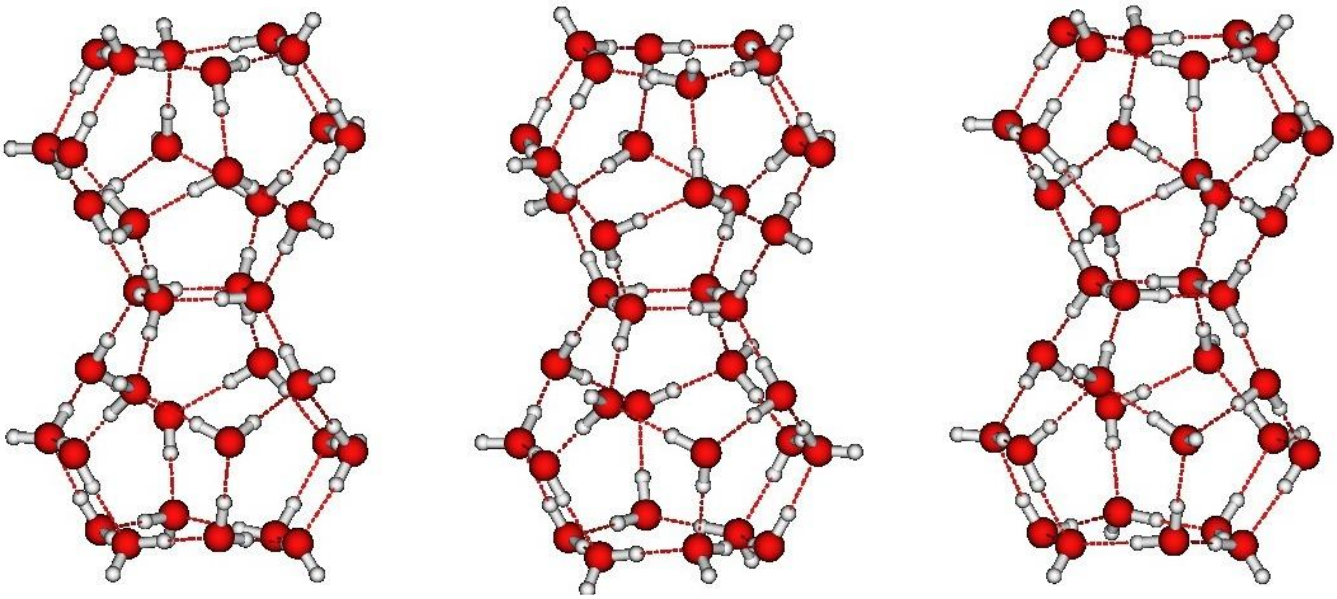


FDI-1
-446.98
(13)

FDI-2
-446.12
(12)

FDI-3
-444.66
(12)

Supplementary Figure 4. Same as in figure 3, for the fused dodecahedral irregular dodecahedral (FDI) cages.



FII-1
-452.74
(14)

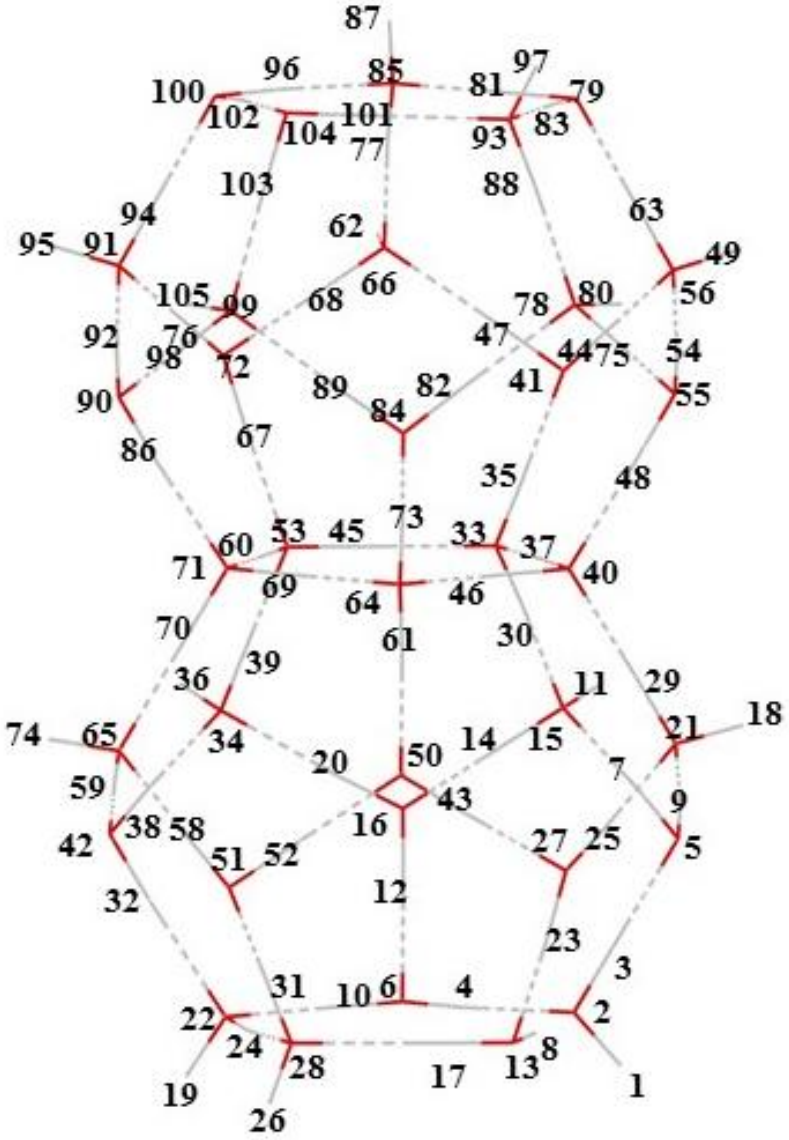
FII-2
-452.58
(12)

FII-3
-443.16
(12)

Supplementary Figure 5. Same as in figure 3, for the fused irregular dodecahedral (FII) cages.

Supplementary Table 2. The Bond Parameters for FDD-1 and FDD-2 cages having the same number of t1d hydrogen bonds.

FDD-1



Cage1:

O100 -H102	0.99584	O100H102...O104	1.7154	O100H102O104	177.37
O100-H96	0.97598	O100H96...O85	1.8973	O100H96O85	176.28
O104-H101	0.97548	O104H101...O93	1.9068	O104H101O93	179.11
O79-H83	0.98135	O79H83...O93	1.8187	O79H83O93	177.77
O79-H81	0.98125	O79H81...O85	1.8158	O79H81O85	179.15
O90-H92	0.9825	O90H92...O91	1.8148	O90H92O91	177.15
O99-H98	1.01582	O99H98...O90	1.5976	O99H98O90	179.87
O84-H89	0.98367	O84H89...O99	1.8034	O84H89O99	176.86
O84-H82	0.97845	O84H82...O78	1.8739	O84H82O78	178
O78-H75	1.02438	O78H75...O55	1.5601	O78H75O55	179.4
O55-H54	0.9826	O55H54...O56	1.8129	O55H54O56	176.74
O41-H44	0.98142	O41H44...O56	1.8329	O41H44O56	176.17
O41-H47	0.97944	O41H47...O66	1.8596	O41H47O66	177.79
O66-H68	1.02775	O66H68...O72	1.5484	O66H68O72	178.96
O72-H76	0.98548	O72H76...O91	1.7863	O72H76O91	179.3
O71-H69	0.99546	O71H69...O64	1.699	O71H69O64	177.37
O40-H46	0.99672	O40H46...O64	1.6903	O40H46O64	179.67
O40-H37	0.99611	O40H37...O33	1.6947	O40H37O33	178.58
O53-H45	0.99634	O53H45...O33	1.6951	O53H45O33	179.5
O53-H60	0.99597	O53H60...O71	1.7001	O53H60O71	178.93

INTERLAYERED:

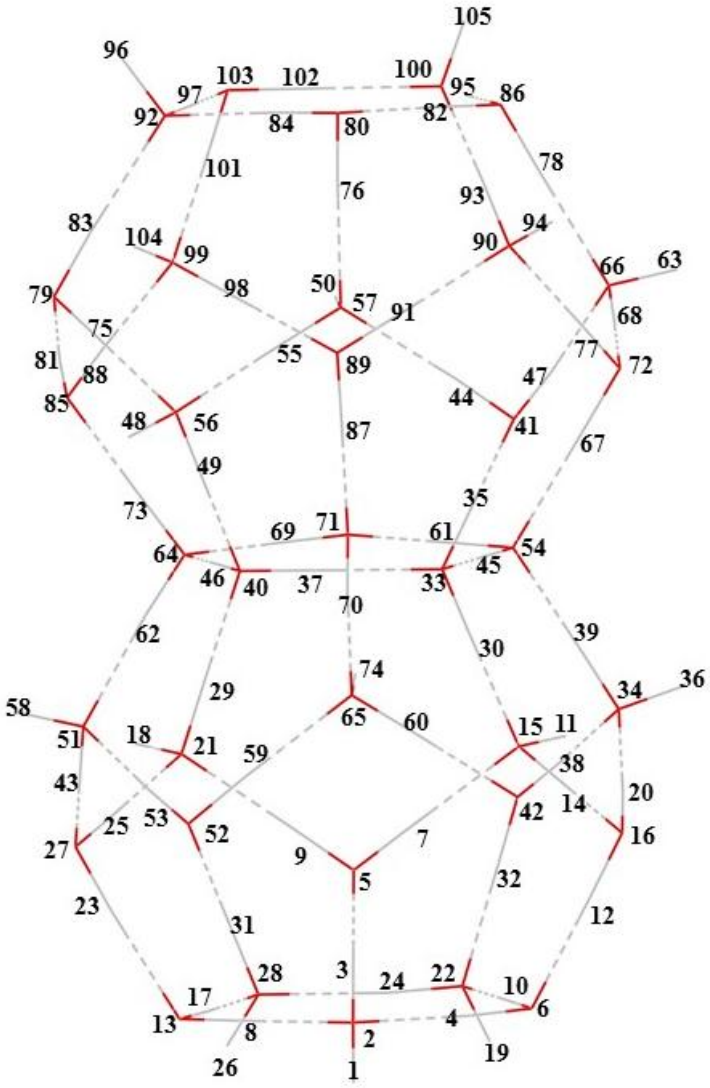
O93-H88	0.99644	O93H88...O78	1.6981	O93H88O78	175.53
O85-H77	0.99703	O85H77...O66	1.6936	O85H77O66	174.96
O91-H94	1.01911	O91H94...O100	1.5786	O91H94O100	179.41
O104-H103	0.98185	O104H103...O99	1.826	O104H103O99	178.74
O56-H63	1.0116	O56H63...O79	1.6129	O56H63O79	179.69
O90-H86	0.98584	O90H86...O71	1.7772	O90H86O71	176.76
O64-H73	1.00456	O64H73...O84	1.6484	O64H73O84	177.73
O55-H48	0.98922	O55H48...O40	1.7526	O55H48O40	178.53
O33-H35	1.00239	O33H35...O41	1.6578	O33H35O41	178.79
O72-H67	0.98822	O72H67...O53	1.7639	O72H67O53	177.88

CAGE-2:

O65-H59	1.01623	O65H59...O42	1.5936	O65H59O42	179
O42-H38	0.98354	O42H38...O34	1.8023	O42H38O34	176.66
O16-H20	0.97824	O16H20...O34	1.872	O16H20O34	177.19
O15-H14	1.02458	O15H14...O16	1.5597	O15H14O16	179.93
O5-H7	0.98239	O5H7...O15	1.8167	O5H7O15	176.76

O5-H9	0.98104	O5H9...O21	1.8286	O5H9O21	175.68
O27-H25	0.9786	O27H25...O21	1.8507	O27H25O21	178.09
O50-H43	1.02647	O50H43...O27	1.5507	O50H43O27	179.17
O51-H52	0.98515	O51H52...O50	1.7898	O51H52O50	177.21
O51-H58	0.98202	O51H58...O65	1.8161	O51H58O65	176.73
O22-H24	0.99617	O22H24...O28	1.6966	O22H24O28	174.88
O6-H10	0.97537	O6H10...O22	1.9112	O6H10O22	178.67
O6-H4	0.98124	O6H4...O2	1.8274	O6H4O2	177.14
O13-H8	0.98103	O13H8...O2	1.8334	O13H8O2	177.7
O13-H17	0.97643	O13H17...O28	1.8904	O13H17O28	178.61
INTERLAYERED:					
O71-H70	0.98608	O71H70...O65	1.7657	O71H70O65	177.82
O64-H61	0.98821	O64H61...O50	1.7534	O64H61O50	175.33
O21-H29	1.00388	O21H29...O40	1.6472	O21H29O40	178.81
O33-H30	0.98979	O33H30...O15	1.7372	O33H30O15	177.81
O34-H39	1.00548	O34H39...O53	1.6435	O34H39O53	179.08
O28-H31	1.01963	O28H31...O51	1.5766	O28H31O51	179.89
O27-H23	0.99615	O27H23...O13	1.7138	O27H23O13	176.93
O2-H3	1.0109	O2H3...O5	1.6177	O2H3O5	179.55
O16-H12	0.99614	O16H12...O6	1.7151	O16H12O6	178.38
O42-H32	0.98197	O42H32...O22	1.8127	O42H32O22	177.73

FDD-2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Cage1

O100-H95	1.03385	O100H95...O86	1.52307	O100H95O86	178.607
O86-H82	0.99697	O86H82...O80	1.70631	O86H82O80	177.611
O80-H84	0.98157	O80H84...O92	1.82689	O80H84O92	177.837
O92-H97	1.01138	O92H97...O103	1.61439	O92H97O103	179.269
O103-H102	0.98053	O103H102...O100	1.83422	O103H102O100	178.638
O99-H98	1.01131	O99H98...O89	1.61726	O99H98O89	179.771
O89-H91	0.97841	O89H91...O90	1.86308	O89H91O90	176.89
O72-H77	0.97954	O72H77...O90	1.84922	O72H77O90	179.254
O66-H68	1.01306	O66H68...O72	1.60915	O66H68O72	178.775
O41-H47	0.98342	O41H47...O66	1.8086	O41H47O66	175.606
O41-H44	0.97848	O41H44...O57	1.85777	O41H44O57	175.029
O57-H55	0.99153	O57H55...O56	1.73096	O57H55O56	174.868
O79-H75	0.97426	O79H75...O56	1.92254	O79H75O56	179.44
O85-H81	0.99214	O85H81...O79	1.74852	O85H81O79	176.622
O85-H88	0.97929	O85H88...O99	1.85602	O85H88O99	177.182
O71-H69	0.99617	O71H69...O64	1.70256	O71H69O64	177.031
O40-H46	1.00506	O40H46...O64	1.64957	O40H46O64	178.56
O54-H45	0.99463	O54H45...O33	1.70712	O54H45O33	179.192
O54-H61	0.99587	O54H61...O71	1.69721	O54H61O71	179.275
O40-H37	1.00182	O40H37...O33	1.66422	O40H37O33	179.446

INTERLAYERED:

O103-H101	0.98404	O103H101...O99	1.79691	O103H101O99	177.498
O90-H93	0.99903	O90H93...O100	1.6794	O90H93O100	175.673
O86-H78	0.98144	O86H78...O66	1.82766	O86H78O66	178.778
O80-H76	0.97529	O80H76...O57	1.90698	O80H76O57	178.318
O79-H83	0.98094	O79H83...O92	1.8333	O79H83O92	176.097
O64-H73	1.01556	O64H73...O85	1.59596	O64H73O85	179.322
O56-H49	1.00792	O56H49...O40	1.63132	O56H49O40	179.475
O33-H35	1.00576	O33H35...O41	1.64201	O33H35O41	179.136
O72-H67	0.987	O72H67...O54	1.77174	O72H67O54	178.032
O89-H87	0.98719	O89H87...O71	1.76633	O89H87O71	177.563

CAGE2:

O27-H25	0.97825	O27H25...O21	1.86076	O27H25O21	179.034
O51-H43	1.02412	O51H43...O27	1.55955	O51H43O27	178.716
O52-H53	0.98515	O52H53...O51	1.78919	O52H53O51	176.491
O52-H59	0.98216	O52H59...O65	1.81267	O52H59O65	176.831
O65-H60	1.0165	O65H60...O42	1.59189	O65H60O42	179.018
O42-H38	0.98346	O42H38...O34	1.80177	O42H38O34	176.382

O16-H20	0.97824	O16H20...O34	1.86431	O16H20O34	177.039
O15-H14	1.02553	O15H14...O16	1.5529	O15H14O16	179.66
O5-H7	0.98297	O5H7...O15	1.8088	O5H7O15	176.74
O5-H9	0.97926	O5H9...O21	1.84278	O5H9O21	175.987
O13-H17	0.97698	O13H17...O28	1.88577	O13H17O28	178.266
O13-H8	0.98069	O13H8...O2	1.83778	O13H8O2	177.814
O22-H24	0.99614	O22H24...O28	1.69693	O22H24O28	174.91
O6-H10	0.97539	O6H10...O22	1.90945	O6H10O22	178.76
O6-H4	0.98103	O6H4...O2	1.82891	O6H4O2	177.044
INTERLAYERED:					
O64-H62	0.98807	O64H62...O51	1.76366	O64H62O51	176.33
O71-H70	0.9864	O71H70...O65	1.76331	O71H70O65	177.504
O34-H39	1.00517	O34H39...O54	1.64113	O34H39O54	179.162
O33-H30	0.99047	O33H30...O15	1.73525	O33H30O15	177.502
O21-H29	1.0002	O21H29...O40	1.67657	O21H29O40	178.246
O27-H23	0.99666	O27H23...O13	1.71132	O27H23O13	177.019
O28-H31	1.02028	O28H31...O52	1.57508	O28H31O52	179.735
O42-H32	0.98199	O42H32...O22	1.81298	O42H32O22	177.527
O16-H12	0.99582	O16H12...O6	1.714	O16H12O6	178.39
O2-H3	1.0092	O2H3...O5	1.62364	O2H3O5	179.995