Supplemental material: Simulation of multi-shell fullerenes using Machine-Learning Gaussian Approximation Potential

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(Dated: August 4, 2022)

Sect. S1. Description of Animations produced for the buckyonion models

To aid visualizing some of the discussions in the paper, we have produced some animations for some buckonion models.

1. BO300_mov.mp4 and BO1374_mov.mp4 files show the buckyonion formation process for BO_{300} and BO_{1374} respectively.
2. BO_growthProcess.mp4 show the clustering and growth process for 540 randomly distributed atoms within a 720-atom fullerene isomer.

Sect. S2. Supporting Tables and Figures

TABLE S1: Ring-size analysis for the buckyonion models.

Models	**Layers**	**Ring size:**				
		5	**6**	**7**	**8**	**9**
$\mathbf{BO}_{60}$	s_1	12	20	0	0	0
$\mathbf{BO}_{300}$	s_1	15	22	3	0	0
	s_2	26	74	14	0	0
$\mathbf{BO}_{540}$	s_1	26	50	12	1	0
	s_2	62	85	28	8	2
$\mathbf{BO}_{840}$	s_1	6	1	0	2	1
	s_2	34	84	20	3	0
	s_3	68	148	40	11	0
$\mathbf{BO}_{1374}$	s_1	27	34	14	3	1
	s_2	25	189	13	2	0
	s_3	50	292	36	3	0
$\mathbf{BO}_{2160}$	s_1	15	20	10	2	1
	s_2	36	291	25	0	5
	s_3	55	380	32	2	5
$\mathbf{BO}_{3774}$	s_1	31	91	17	4	4
	s_2	47	183	26	5	4
	s_3	112	333	80	18	6
	s_4	179	422	123	24	7

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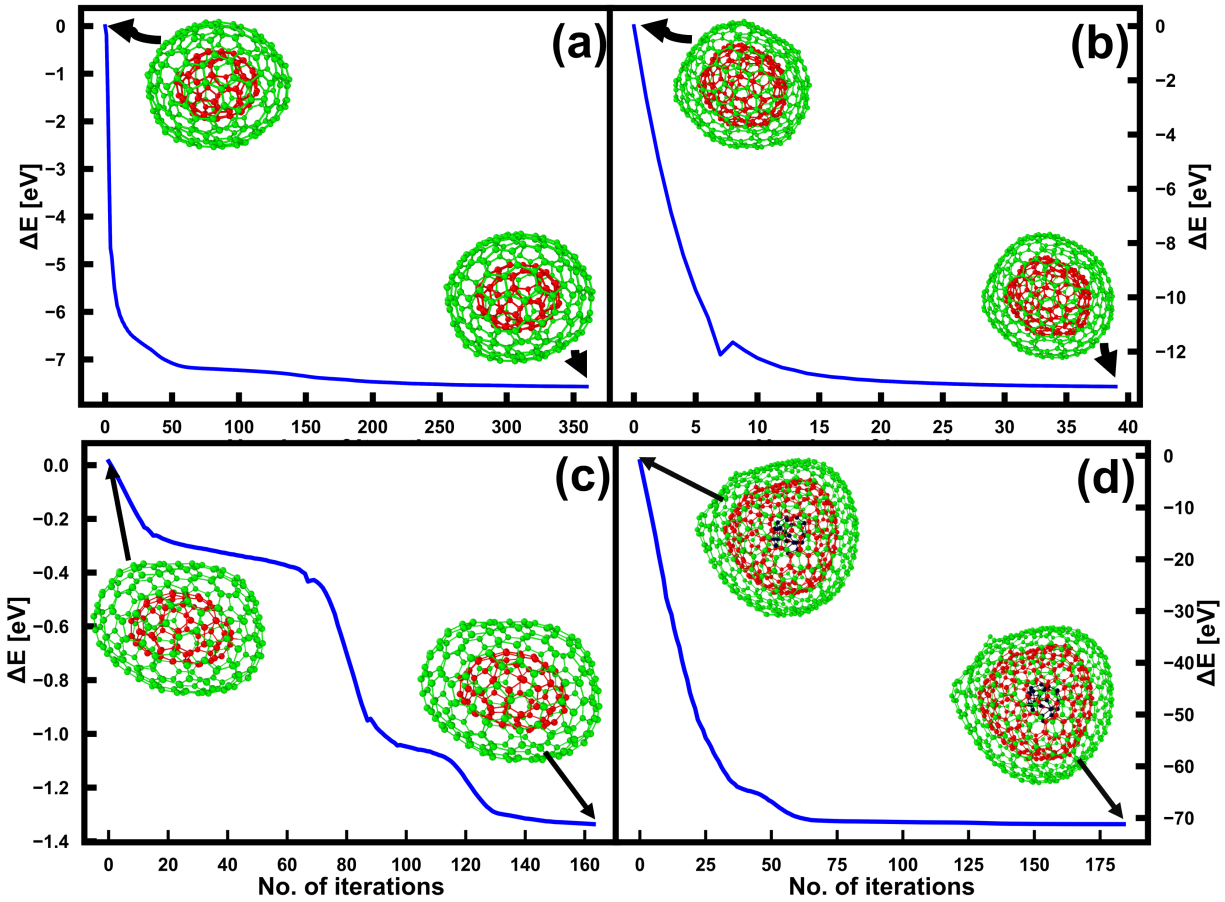

FIG. S1: Plots of the energy difference (ΔE) against the Conjugate gradient (CG) iterations carried out using VASP on BO_{300} (a) and BO_{540} (b). SIESTA was used for the BO_{300} (c) and BO_{840} (d) models as well. The insets in a-d represent the models before and after CG relaxation.

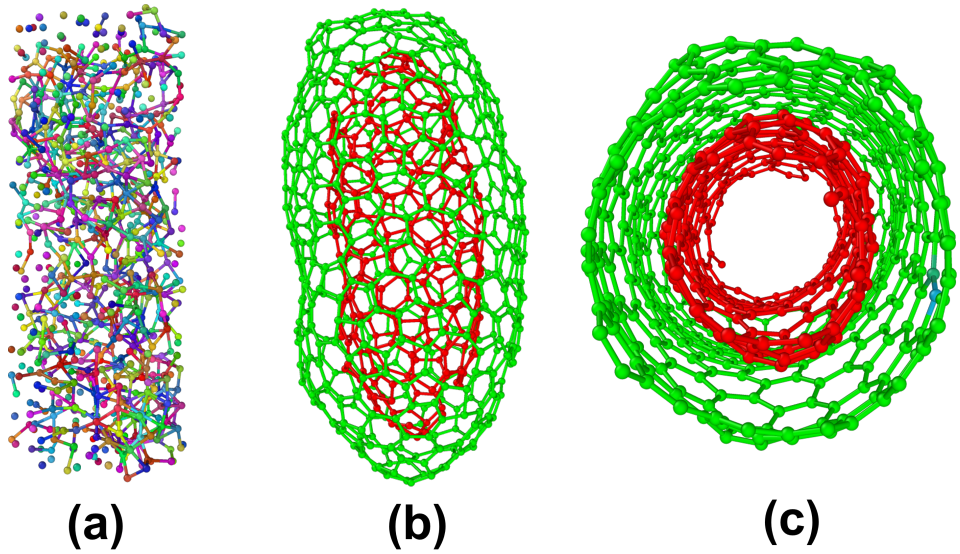

FIG. S2: Starting from (a) an initially random atomic configuration with a cylindrical shape, (b) a capped multi-wall carbon nanotube was formed. The figure in (c) show the nanotube from the z-axis with the cap sliced off. The system has 840 atoms and periodic boundaries only in the z-axis.

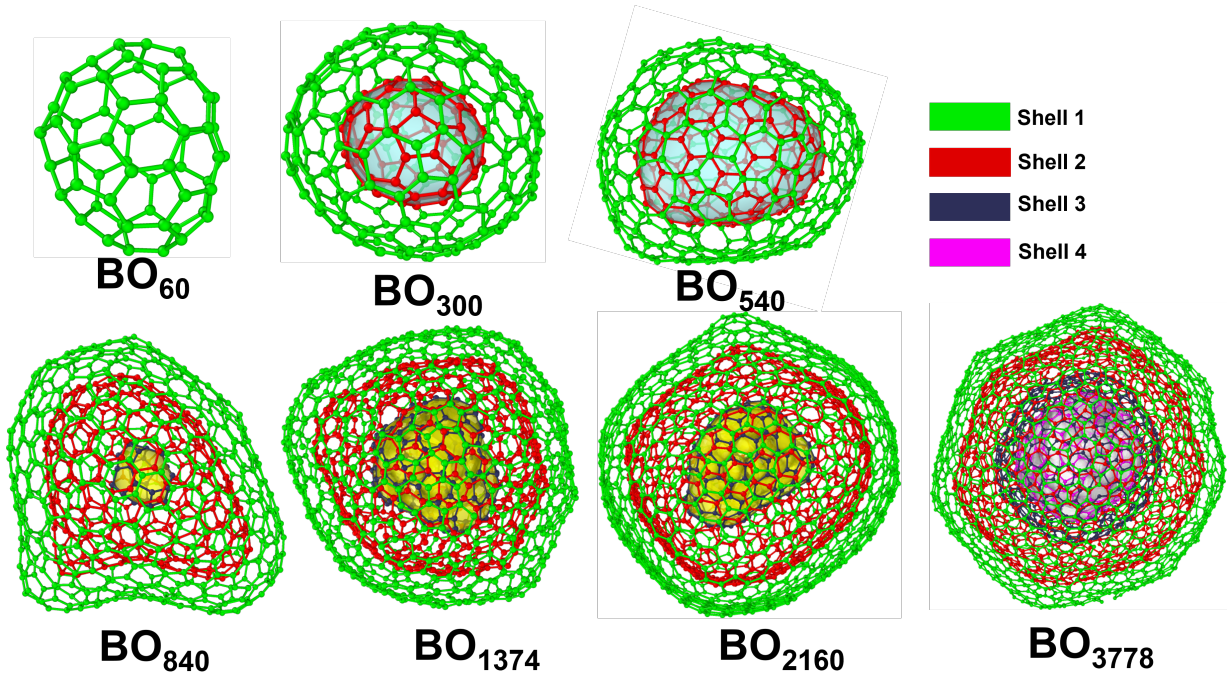

FIG. S3: Figure showing some of the buckyonions models simulated in this work

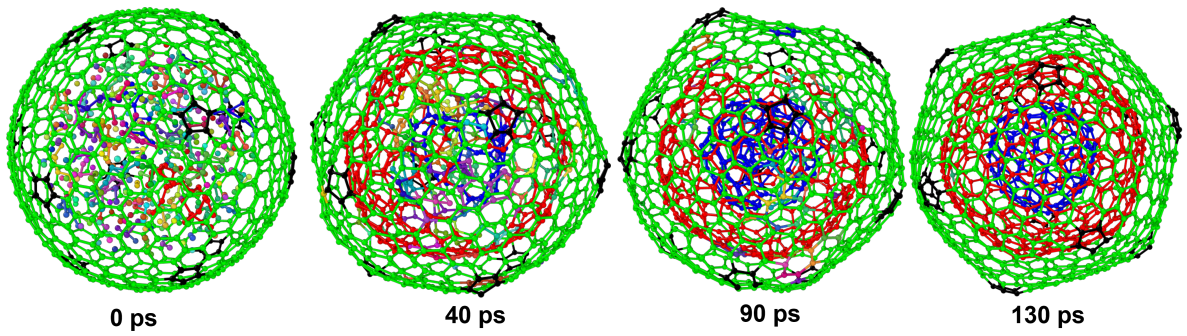

FIG. S4: Growth Process from C_{720} isomer with 540 atoms randomly distributed C atoms. The outermost shell (green) remained with 720 atoms at the end of the simulation. The heptagons in the outermost shell are coloured in black.

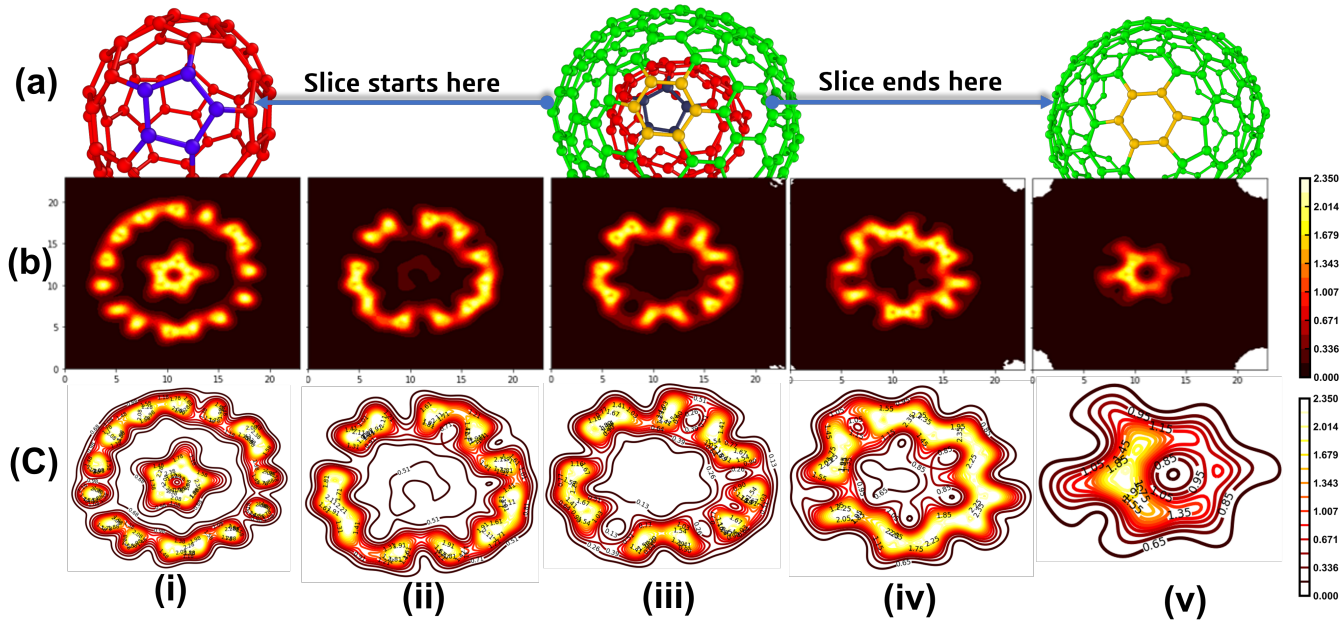

FIG. S5: Figure showing the distribution of the charge density for one end of BO_{300} model in -xy planar-slices starting with a pentagon (blue) in the inner shell (red) in a(i) to the first slice in the outer shell (green) showing a hexagonal structure (yellow) in a(v). The figures in b(i - v) and c(i - v) show the heat-map and contour values of the charge density for 5 slices from a(i) to a(v). The entire system is shown in a(iii) and charge distribution in the other end of the system is discussed in main manuscript.