Supplementary information

for

Polarizability as a tool to determine the electrostatic shielding effect of nanocarbon cages: A polarizability distribution study on noble gas endohedral fullerenes

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Table S3 The radii of the uniform-field zone and the field penetration factors p at the fullerene centers computed at M06-2X/SVP level.

Fig. S1 Electron density differences (EDDs) between carbon cages with and without NG encapsulation for NG@C_{40}. Red denotes the largest decrease in electron density, while blue denotes the largest increase in electron density. The color scale was set in range between -0.001 au and 0.001 au for left, -0.002 au and 0.002 au for right.

Fig. S2 Electron density differences (EDDs) between carbon cages with and without NG encapsulation, calculated at LC-BLYP/SVP and PBE[62]/SVP level, respectively. Red denotes the largest decrease in electron density, while blue denotes the largest increase in electron density. For C_{40} and C_{60} complexes, the color scale was set in range of -0.0002 au to 0.0002 au. For C_{180} complexes, the color scale was in range of -0.00004 au to 0.00004 au.

Fig. S3 Variations in p(NG) calculated from eq. 6, and p from eq. 5, with cage size (n) at PBE/SVP level (top) and LC-BLYP/SVP level (bottom).

Table S1 Variation of α(NG@C_n) and p(NG) with cage size respectively computed at different level.

`	He@C_n			Ar@C_n		
n	α(NG@C_n)	α^P(NG)	p(NG)	α(NG@C_n)	α^P(NG)	p(NG)
			M06-2X/SVP			
40	317.73	0.04	3.1	321.90	0.59	5.4
50	403.55	0.10	7.4	406.18	0.96	8.7
60	487.63	0.21	14.8	489.33	1.38	12.6
70	606.93	0.17	11.6	608.20	1.25	11.3
80	736.03	0.14	9.8	736.87	1.11	10.1
90	811.40	0.27	19.1	812.33	1.85	16.9
100	943.85	0.23	16.2	944.84	1.90	17.3
116	1249.67	0.13	9.2	1249.85	0.78	7.1
132	1269.46	0.38	26.9	1270.49	2.87	26.2
144	1453.87	0.35	24.7	1454.69	2.66	24.2
180	1852.79	0.42	29.6			
			M06-2X/TZVP			
40	349.72	0.07	4.7	351.84	0.71	6.5
50	441.06	0.12	8.6	442.48	1.09	9.9
60	528.95	0.21	14.4	530.49	1.53	14.0
70	654.45	0.19	13.1	655.78	1.39	12.7
80	789.25	0.14	10.2	790.07	1.24	11.3
90	867.55	0.23	16.4	868.89	2.03	18.5
			LC-BLYP/SVP			
40	311.58	0.06	3.7	315.68	0.61	5.6
50	393.42	0.14	8.7	396.23	1.03	9.4
60	474.42	0.22	14.4	476.44	1.49	13.7
70	588.55	0.22	14.5	590.05	1.49	13.7
80	718.43	0.18	11. 8	719.31	1.26	11.5
90	785.53	0.33	21.6	786.65	2.20	20.2
100	1001.28	0.18	11.6	1002.10	1.17	10.8
116	1280.02	0.09	5.8	1280.18	0.55	5.1
132	1221.35	0.47	30.7	1222.58	3.21	29.5
144	1400.96	0.44	28.4	1401.95	3.00	27.6
180	1777.59	0.52	33.5			
			LC-BLYP/TZVP			
40	342.04	0.08	5.4	344.75	0.75	6.9
50	428.98	0.16	10.3	430.91	1.16	10.6
60	513.85	0.24	15.6	515.61	1.63	15.0
70	633.63	0.24	15.6	635.02	1.63	14.9
80	768.67	0.20	13.1	769.39	1.40	12.8
90	839.39	0.34	22.1			

Table S2 The average radius r for cages, the inner and outer radii of the shells (a, b), HOMO-LUMO gaps (E_{gap}), ε, mean polarizability ($<\alpha>$) , local (α^P) and charge transfer (α^P) contributions for C_n at M06-2X/SVP level, and the polarizabilities (field penetration p) predicted with Penn's models.

n	r(Å)	a(Å) [a]	b(Å) [b]	E_{gap}(au)	ε [c]	$<\alpha>$ (au)	α^P(au)	α^Q(au)	Penn
40	2.91	2.01	3.81	0.13	30.87	316.8	89.1	227.7	343.1(16.0)
50	3.25	2.35	4.15	0.11	47.23	403.0	105.4	297.6	454.9(11.1)
60	3.55	2.65	4.45	0.16	21.43	487.3	121.3	366.0	522.4(23.9)
70	3.84	2.94	4.74	0.15	24.25	606.6	139.3	467.3	635.6(22.0)
80	4.11	3.21	5.01	0.08	94.87	735.8	156.5	579.3	822.4(6.3)
90	4.35	3.45	5.25	0.11	44.34	811.0	171.4	639.6	908.4(13.3)
100	4.59	3.69	5.49	0.09	70.00	943.7	188.7	755.0	1061.4(8.8)
116	4.93	4.03	5.83	0.09	64.78	1249.6	219.9	1029.7	1267.6(9.9)
132	5.26	4.36	6.16	0.13	32.80	1269.3	236.0	1033.3	1404.3(19.2)
144	5.50	4.60	6.40	0.11	44.41	1453.7	257.1	1196.6	1616.8(14.9)
180	6.14	5.24	7.04	0.13	30.71	1852.7	310.7	1542.0	2055.7(22.1)

[a] $a = r-\Delta$, [b] $b = r+\Delta$, Δ = 0.9 Å.[c] $\varepsilon \approx 1 + (E_p/E_{gap})^2$, E_p = 20 eV

Table S3 The radii of the uniform-field zone R and the field penetration factors p at the fullerene centers computed at M06-2X/SVP level.

	R(Å)			p(×100%)			
n	x	y	z	x	y	z	p
40	1.0	1.0	1.3	16.0	22.7	21.9	20.2
50	1.5	1.5	0.8	26.3	26.3	18.6	23.7
60	1.5	1.5	1.5	26.4	26.4	26.4	26.4
70	1.8	1.8	2.0	20.7	20.7	25.4	22.3
80	1.5	1.5	2.8	15.6	15.6	23.0	18.1
90	2.5	2.0	2.5	24.0	24.8	26.4	25.1
100	2.5	2.5	2.5	21.6	23.9	22.6	22.7
116	3.0	3.0	3.0	10.7	10.7	10.7	10.7
132	3.0	3.0	4.5	28.8	28.8	29.4	29.0
144	3.5	3.5	2.8	24.2	24.1	28.7	25.7
180	4.0	4.0	4.0	29.7	29.7	29.7	29.7

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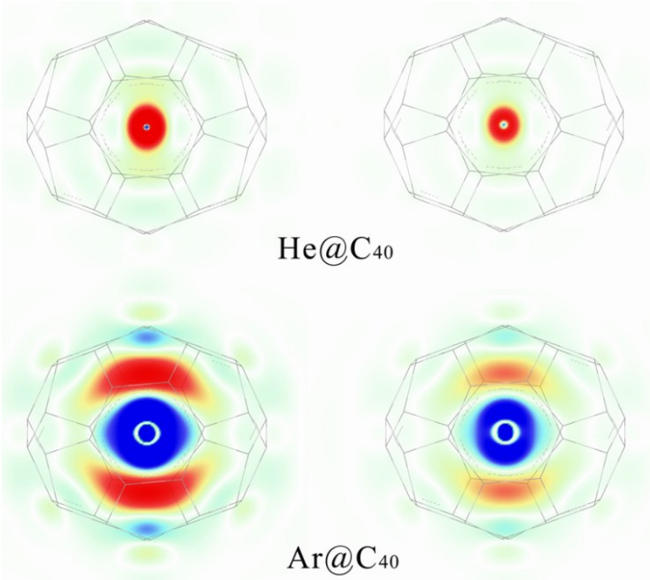

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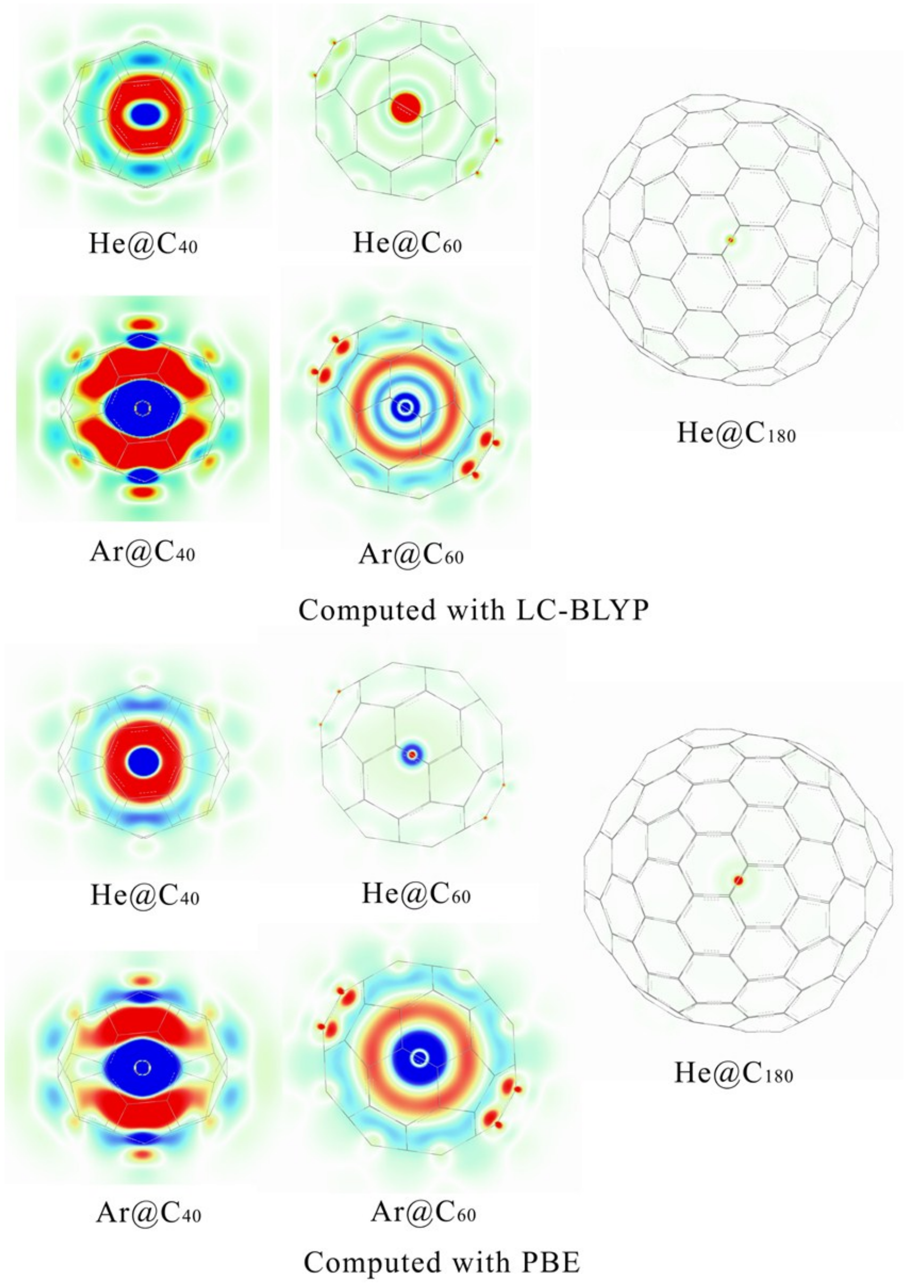

62. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865-3868.

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