Electronic Supplementary Material (ESI) for Analyst.

Supplementary data:

Interrupting flux of delocalized electrons on the dibenzo-18-crown-6-embedded graphite sheet and its relative counteraction in the presence of potassium ions

Mojtaba Shamsipur, Avat (Arman) Taherpour and Afshin Pashabadi*

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Computational studies on structures of the DB18C6 and the complexes 1:1 and 2:1 of ligand with K^+

The calculations on the structures of the DB18C6 and the complexes 1:1 and 2:1 of ligand with K^+ (complexes [DB18C6].K^+ and $[DB18C6]_2.K^+$) were made by the appropriate QM-DFT methods. The structures of the ligand (**I**) and the complexes were optimized by DFT-B3LYP/6-31G* method [14]. The results of the selected structural data for the ligand (**I**) and the complexes [DB18C6].K^+ and $[DB18C6]_2.K^+$, *i.e.* bond lengths (in Å), bond angles (in °) and the point groups were determined and shown in the Figure S1A for ligand, Figure S1B for complex [DB18C6].K^+ and Figure S1C for complex $[DB\text{-}18\text{-}C6]_2.K^+$. The HOMO and LUMO orbital shapes and electrostatic charges of the ligand DB18C6 and the complexes 1:1 and 2:1 of ligand with K^+ (complexes [DB18C6].K^+ and $[DB18C6]_2.K^+$) are shown in Figure S2A, S2B and S2C. Table S1 shows the selected structural data of the ligand DB18C6 and complexes of the ligands with K^+. The optimized structures of the complexes by B3LYP/6-31G* method demonstrated that the point groups of the complexes are: [DB18C6].K^+ (C_1) and $[DB18C6]_2.K^+$ (D_2). The ligand DB18C6 was attracted around the K^+ ion at the complexes 1:1 and 2:1 of ligand with K^+ (complexes [DB18C6].K^+ and $[DB18C6]_2.K^+$). The energy of the HOMO-LUMO gap of the complexes [DB18C6].K^+ and $[DB18C6]_2.K^+$ were calculated: 5.60 and 5.84eV, respectively. The lowest and highest O-K^+ bond lengths in the complexes [DB18C6].K^+ and $[DB18C6]_2.K^+$ are: [2.754 & 2.781] and [3.054 & 3.190] Å, respectively. The dipole moments of the complexes [DB18C6].K^+ and $[DB18C6]_2.K^+$ are: 1.26 and 0.02 Debye, respectively.

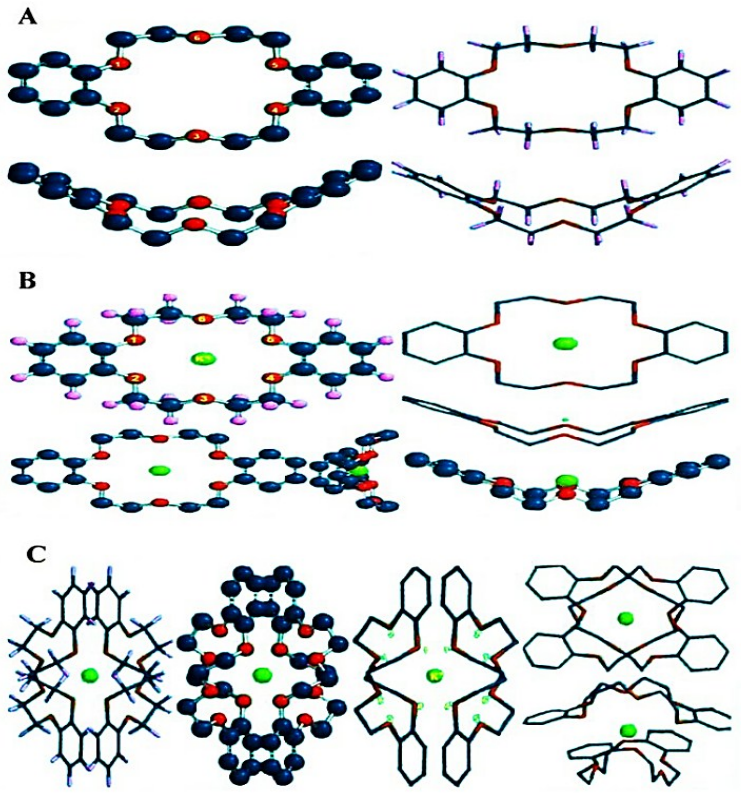

Fig. S1. (A) The optimized structure of the ligand DB18C6 by B3LYP/6-31G* method. The point group is C_2v. (B) The optimized structure of the complex (1:1) of the ligand DB18C6 and K^+ by B3LYP/6-31G* method. The point group is C_2. (C) The optimized structure of the complex (2:1) of the ligand DB18C6 and K^+ by B3LYP/6-31G* method. The point group is D_2.

Table 1. The selected structural data of the ligand and complexes 1:1 and 2:1 of the ligand DB18C6 with K^+.

Selected data	Ligand-I (DB18C6)	$[DB18C6]_1.K^+$	$[DB18C6]_2.K^+$
Point group	C_{2v}	C_2	D_2
Bond length (Å)			
O1-O2	2.584	2.602	2.674
O1-O3	4.802	4.675	3.715
O1-O4	5.540	5.459	4.948
O1-O5	4.900	4.799	5.006
O1-O6	2.900	2.794	2.814
O3-O6	5.671	5.402	4.263
O1-O1’	-	-	4.153
O2-O2’	-	-	4.153
O3-O3’	-	-	5.078
O4-O4’	-	-	4.153
O5-O5’	-	-	4.153
O6-O6’	-	-	5.078
O1-K	-	2.754	3.139
O2-K	-	2.754	3.054
O3-K	-	2.781	3.190
O4-K	-	2.754	3.139
O5-K	-	2.754	3.054
O6-K	-	2.781	3.190
O1’-K	-	-	3.054
O2’-K	-	-	3.139
O3’-K	-	-	3.190
O4’-K	-	-	3.054
O5’-K	-	-	3.139
O6’-K	-	-	3.190
Bond angle (°)			
O1KO2	-	56.38	51.14
O1KO3	-	115.27	100.65
O1KO4	-	164.68	149.78
O1KO5	-	121.21	107.85
O1KO6	-	60.62	55.06
O1’KO2’	-	-	51.14
O1’KO3’	-	-	100.65
O1’KO4’	-	-	149.78
O1’KO5’	-	-	107.85
O1’KO6’	-	-	55.06
Energy data			
E_{HOMO} **(eV)**	-5.26	-8.53	-8.13
E_{LUMO} **(eV)**	0.52	-2.93	-2.29
$\Delta E_{HOMO\text{-}LUMO}$ **(eV)**	5.78	5.60	5.84
Hardness (η)	2.89	2.80	2.92
Dipole moment (D)	1.90	1.26	0.02
ΔG_f **(**kcal.mol^{-1}**)**	-	-76.46	-99.09

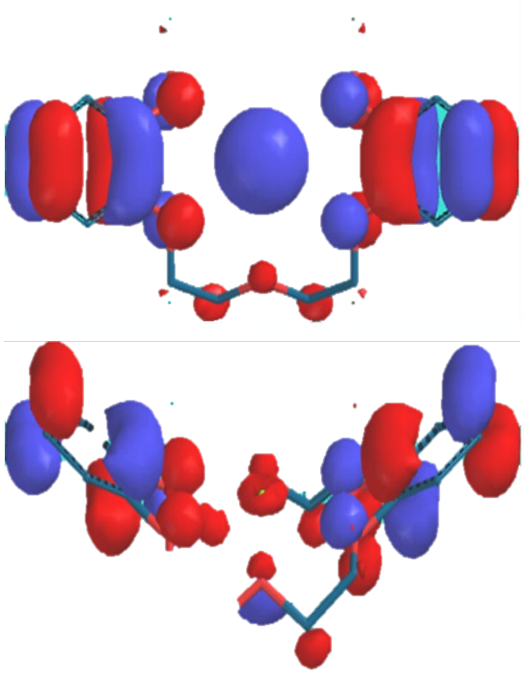

Fig. S2. The HOMO-LUMO interactions between ligand [DB18C6] and K^+ ion.

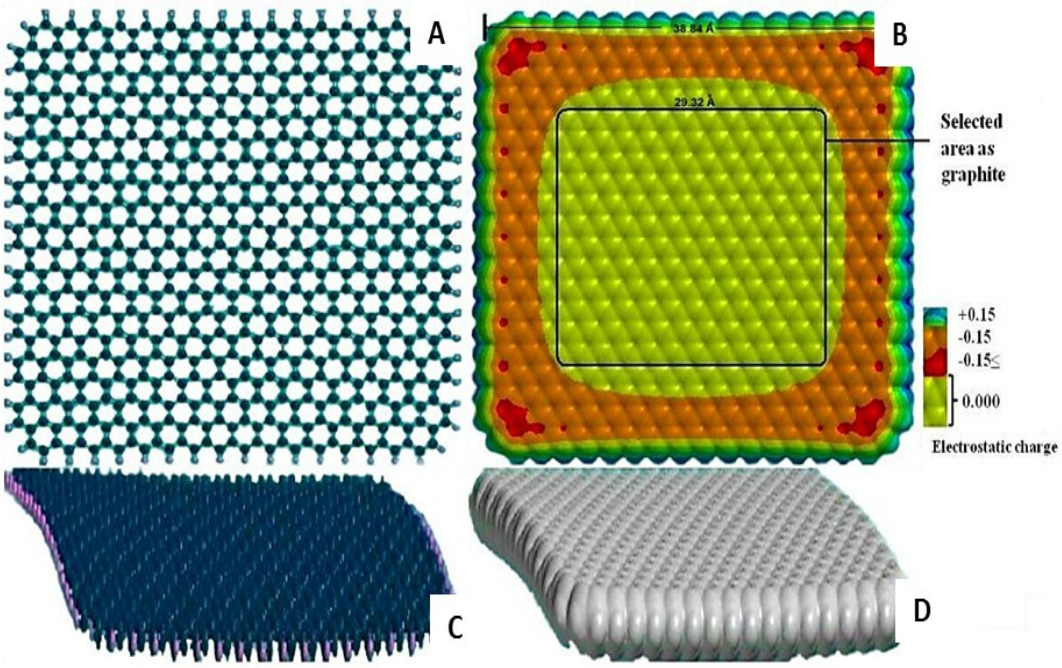

Fig. S3. The calculated model of graphene surface by molecular mechanics MMFF94 method. **A)** Ball and spoke model, surface form, **B)** Ball and spoke model, side form, **C)** Electrostatic potential model with natural charges and **D)** Electron density model. In (C) has shown a quadrangle (with dimensions 38.84x38.84 Å). The main area (yellowish area) as graphite has demonstrated in (C) with dimensions 29.32x29.32 Å. This area has selected for the modeling. The electrostatic charge on carbon atoms is 0.000 in this selected area.