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PHYSICAL METHODS OF INVESTIGATION

Interaction of Na, Mg, Al, Si with Carbon Nanotube (CNT): NMR and IR Study[1]

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Abstract—A Quantum Mechanics (QM) is used for investigated the nature of metals transport and interaction with single-walled carbon nanotubes (SWCNTs) inter membranes. Metal species can be transported actively by a combination of SWCNT-membranes conducting channels that have been used for bio-molecular and detection. This study is based on the interaction of Na, Mg, Al, and Si with the structural features of SWCNTs in the ground state ab initio, HF theory and DFT calculation have been performed with the program Gaussian A7 package suite of programs. We used HF and DFT (B3LYP) method for calculation energy, chemical shift nucleus magnetic resonance and proportion thermodynamic by DFT-IR and DFT-NMR for RWCNT in absence and presence metals. The basis set used 6-31G and 6-31G* that increasing electronegativity metals increased the total energy. The proportion SWCNTs were changed by them. In this study presented a comprehensive on effects of metals on SWCNTs, which are on theirs electronic structure, and transfer of charge from metal to SWCNTs. The results are presented for T = 310 K, the temperature of human's body.

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INTRODUCTION

Single-Walled Carbon Nanotube (SWCNT) Structure

Carbon nanotubes are quasi one-dimensional objects and may be derived from graphite sheets [1]. In this study, only open ended, single-walled carbon nanotubes (SWCNTs) will be considered. These single-walled carbon nanotubes (hereafter referred to only as SWCNTs) are composed of (benzene-like) hexagons and therefore are expected to be highly aromatic structures [2]. Single-walled carbon nanotubes (SWCNT) are constructed of a single sheet of graphite (diameter 0.4–2 nm) [3]. One of the major areas of CNT research is the field of biomedical materials and devices. Many applications for CNT have been proposed including biosensors, drug, and vaccine delivery vehicles and novel biomaterials [4].

SWCNTs can be chiral or nonchiral, again depending on the way of the rolling up vector Fig. 1, $C = na_1 + ma_2 = (n, m)$, where a_1 and a_2 are the primitive lattice vectors of the graphene and n, m are integers [5, 6]. SWCNTs are classified into three types namely, armchair (n, n) nanotubes, zigzag (n, 0) nanotubes, and chiral (n, m) nanotubes with $n \neq m$ [7].

However, before such materials can be incorporated into new and existing biomedical devices, the toxicity and biocompatibility of CNT needs to be thoroughly investigated. For the purposes of this review, biocompatibility will be defined as "the ability of a material to perform with an appropriate host response in a specific application" [8].

This work, we use SWCNTs (100–120) from kind of armchair carbon nanotubes (5, 5) and (6, 6) that shows in Fig. 2. Numerous electrical measurements on SWCNT ensembles have revealed that chemical doping by donors (Li, K, Cs, or Rb) or acceptors (Br_2, I_2, or acids) decreases the room temperature electrical resistance by up to two orders of magnitude at saturation doping [9–11]. The important problem is metals passing through cells membrane. Because, there are barriers

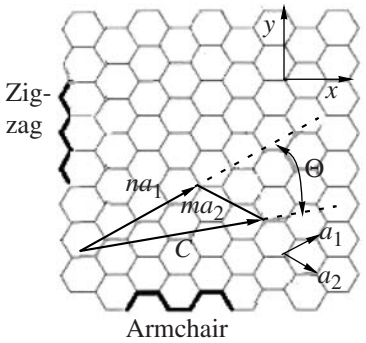

Fig. 1. Schematics of the generation of a carbon nanotube by folding a section of a graphene sheet.

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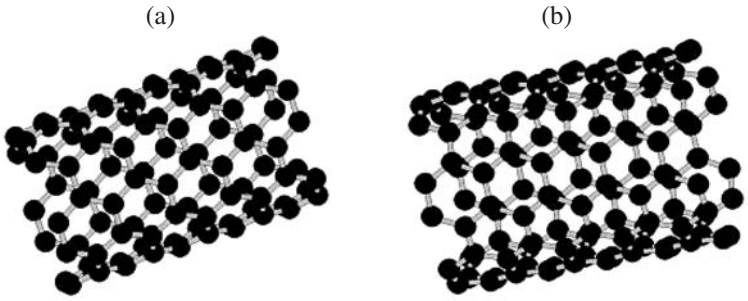

Fig. 2. The optimized configuration Side-view SWCNT: C_{100} (a) and C_{120} (b).

for them passing through protein canals in cells membrane. Additionally, upon interaction, changes in activity, stability, and solubility ions compatibility may occur in cells. A lot of studies are for replacing protein canals into cells membrane for passing proteins, drug and ions of metal.

Therefore the presence of the SWCNT and its consequences to the biological activity of ions metal are of high impact in the development of biosensors, immunoassays and drug delivery systems [12, 13]. This work, we used armchair carbon nanotube (5, 5) and (6, 6). Indeed, vibrational frequencies of finite-length carbon nanotubes were recently examined [14] and another result of 319.9 cm^{-1} is consistent with oscillations along the radial directions (radial modes), although it cannot be assessed accurately due to the sensitivity to the number of rings [15]. We suggest that SWCNT intercalate into cells membrane replacing protein canals and are studying passing metal ions (Na, Mg, Al, and Si) in length of SWCNT by Quantum Mechanics (QM).

COMPUTATIONAL DETAILS

Geometry Optimization Quantum Mechanics

The geometry optimizations were performed using an all-electron linear combination of atomic orbitals Hatree–Fock (HF) and density functional theory (DFT) calculations using the Gaussian A7 package. We are interested in the structural features of single-walled carbon nanotube (SWCNT) in the ground state an atomic and amino acids (His and Ser). In HF theory the energy has from:

$$E_{\mathrm{HF}} = \nu + \langle hp \rangle + 1/2 \langle P_j(\rho) \rangle - 1/2 \langle P_k(\rho) \rangle, \quad (1)$$

where ν is the nuclear repulsion energy, ρ is the density matrix, $\langle hp \rangle$ is the one electron (kinetic plus potential) energy. $1/2 \langle P_j(\rho) \rangle$ is the classical coulomb repulsion of the electrons and $-1/2 \langle P_k(\rho) \rangle$ is the exchange energy resulting from the quantum (fermions) nature of electrons.

In density function theory the exact exchange (HF) for a single determinant is replaced by a more general expression the exchange correlation functional, which can include terms accounting for both exchange energy and the electron correlation, which is omitted from Hartree–Fock theory:

$$E_{\mathrm{KS}} = \nu + \langle hp \rangle + 1/2 \langle P_j(\rho) \rangle + E_{\chi(\rho)} + E_{C(\rho)}, \quad (2)$$

where, $E_{\chi(\rho)}$ is the exchange function and $E_{C(\rho)}$ is the correlation functional. The correlation function of Lee, Yang, and Parr is includes both local and non-local term [16]. The optimizations of solids are carried out including exchange and correlation contributions using Beckê̂s three parameters hybrid [17, 18] and Lee–Yang–Parr (LYP) correlation [B3LYP]; including both local and non-local terms with the program Gaussian A7 package.

Compared to Raman spectroscopy, much less information about the vibration properties of carbon nanotubes can be gained from IR spectra. This limitation mainly results from the strong absorption of SWCNTs in the IR range.

Accurate predictions of molecular response properties to external fields are of general significance in various areas of chemical physics. This especially refers to the second-order magnetic response properties (NMR), since the magnetic resonance based techniques have gained substantial importance in chemistry and biochemistry that NMR data shown with two parameters isotropic (σ_{iso}) and an isotropic (σ_{aniso}) shielding. In the present paper, we report a HF and density functional study of isotropic ^{13}C and ^{1}H chemical shifts for SWCNTs with Na, Mg, Al, and Si.

RESULTS AND DISCUSSION

The B3LYP and HF by 6-31G and 6-31G* calculation for the molecular SWCNT models considered were validated by the calculated NMR shifts and thermodynamic properties of an open-ended SWCNT (5, 5) and (6, 6) molecular systems.

Table 1. The total energy calculated in various basis set at HF & B3LYP for SWCNTs (5.5) and (6.6) with ions metal Na, Mg, Al and Si

Energy total (Hartree)		Na				Mg		Al		Si	
		HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP
C_{100}	6-31G	–2241.98	–2256.53	–2401.83	–2416.63	–2438.87	–2453.67	–2480.80	–2495.72	–2527.27	–2542.30
(5.5)	6-31G*	–2269.16	–2284.21	–2430.75	–2446.16	–2468.15	–2483.58	–2510.66	–2526.16	–2557.67	–2573.29
C_{120}	6-31G	–2990.32	–3009.391	–3150.15	–3169.61	–3187.08	–3206.55	–3229.18	–3248.72	–3275.58	–3295.37
(6.6)	6-31G*	–3026.37	–3046.26	–3188.02	–3208.34	–3225.34	–3245.70	–3267.95	–3288.37	–3315.00	–3335.57

Table 2. Calculated thermal energy, thermal enthalpy, total enthalpy, thermal entropy, thermal Gibbs free energy, Gibbs free energy, and heat capacity by IR-HF/6-31G

	Cv_{th} (cal/mol)	S_{th} (cal/mol)	H_{th} (cal/mol)	G_{th} (cal/mol)	E_{th} (cal/mol)
$SWCNT_{100}$(5.5)	104.25	146.61	245.64	201.93	245.05
$SWCNT_{100}$-Na	103.13	139.32	262.12	220.60	261.68
$SWCNT_{100}$-Mg	103.44	138.53	255.49	214.21	255.04
$SWCNT_{100}$-Al	105.85	142.81	247.06	204.50	246.61
$SWCNT_{100}$-Si	105.58	143.55	243.11	200.33	242.65

Total Energy

The total energy (E_{total}) of this interaction is listed in Table 1, which the E_{total} increase to converge with an increasing carbon number. In this study the metals on the center of a hexagon (HC) and muse are related to competitive interactions between ions metal and SWCNTs. We investigate the structural electronic and magnetic properties their. The most stable configuration for Si adsorbed on SWCNTs is also at the (HC) site at competitive another atoms of SWCNT because the electro negativity is the most great. The calculated amounts of Dipole, Quadrupole, Octapole, and Hexadecapole moments at the HF and B3LYP levels in various basis set are given in Table 2. Hybridizing Coefficient is different in various methods and basis set.

NMR Data

Calculations of the NMR shifts with the magnetic field perturbation method of GIAO (gauge in dependent atomic orbital) incorporated with the program Gaussian A7 package. The results of the calculations for the carbon nearest neighbors' atoms in SWCNTs are presented in Table 3. The calculated magnetic shielding in Figs. 3, 4 was converted into σ_{iso}, σ_{aniso} chemical shifts by ^{13}C absolute shielding in SWCNT (5, 5). They are worth noting that the last approach leads to a substantial improvement in the calculated magnetic properties. Regarding the method for achievement of gauge invariance for the present case, at the B3LYP and HF levels on the other hand at the hybrid B3LYP level, GIAO is found to be slightly superior.

IR Data

The calculated infrared is for C_{100} at HF/6-31G with Na, Mg, Al, and Si. They showed in Table 2. The properties thermodynamic are decrease with increase electro negativity atoms.

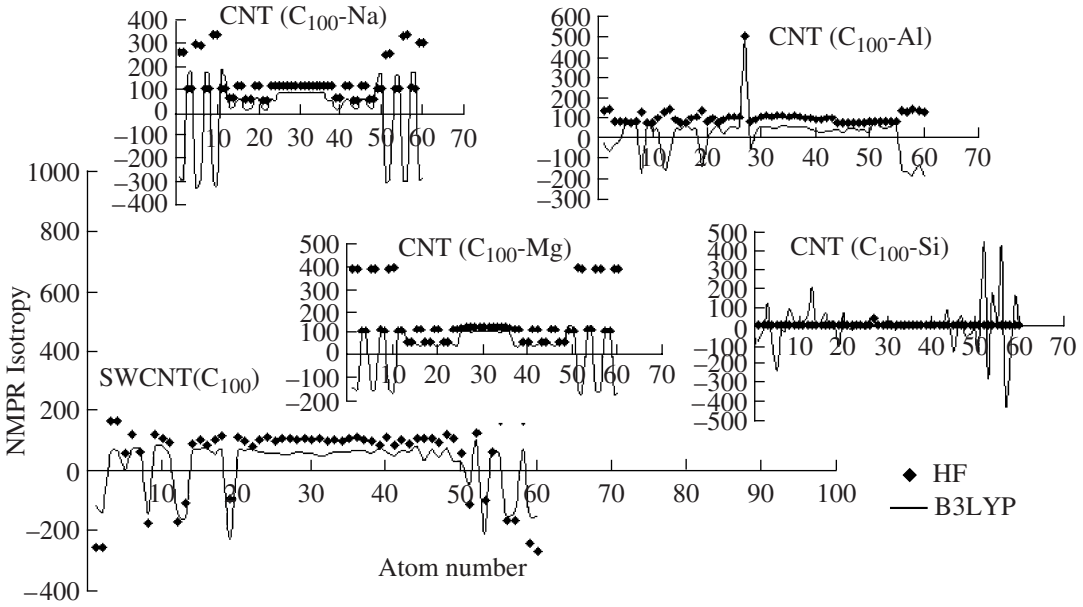

Fig. 3. NMR isotropy diagrams of SWCNT (C_{100}) for HF/6-31G (◆) and BLYP/6-31G (–) method.

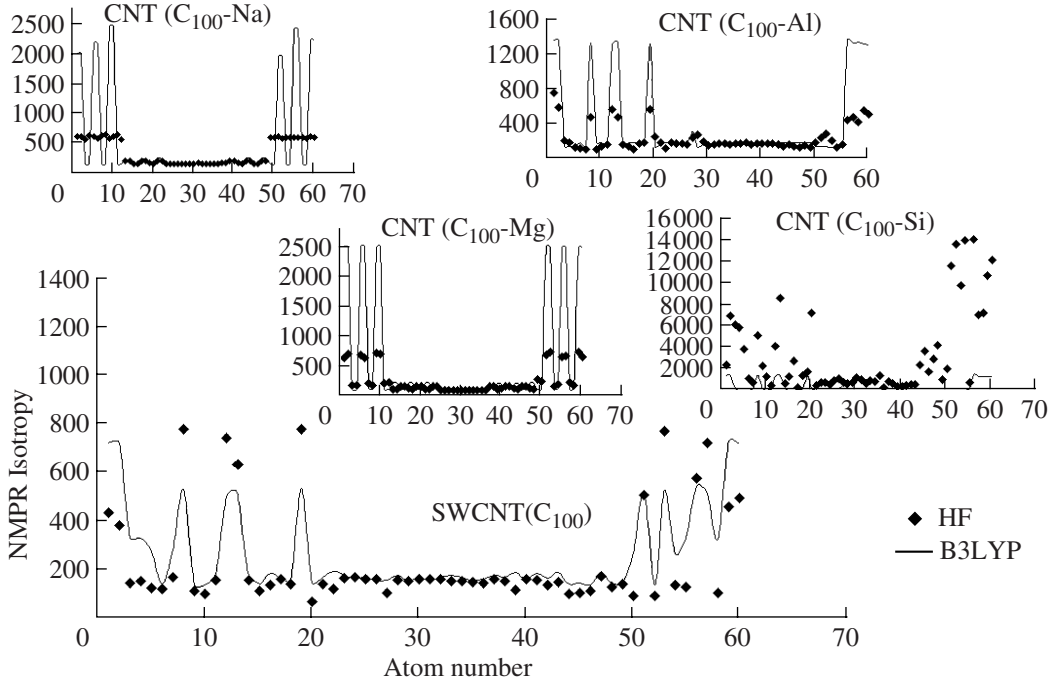

Fig. 4. NMR anisotropy diagrams of SWCNT (C_{100}) for HF/6-31G (◆) and BLYP/6-31G (–) method.

CONCLUSIONS

Ab initio calculations using DFT/B3LYP and HF levels with 6-31G and 6-31G* basis set of theory have allowed the determination of structure electronic, properties thermodynamic, magnetic properties for SWCNTs with Na, Mg, Al, and Si. NMR chemical shielding tensors in the methods framework makes it possible to study the chemical shift of specific group in carbon nanotubes. In this study presented a comprehensive on effects of atoms on SWCNTs that it is on its electronic structure: 1) transfer of charge from the atom to the SWCNTs; 2) electrostatic interactions between the delocalized π electrons of the SWCNTs and atoms.

Table 3. Calculation Dipole, Quadrupole, Octapole and Hexadecapole moments calculated in various basis sets at HF and B3LYP for $C_{100}(5,5)$, $C_{120}(6,6)$

			$SWCNT_{100}$		$SWCNT_{100}$-Na		$SWCNT_{100}$-Mg		$SWCNT_{100}$-Al		$SWCNT_{100}$-Si	
			HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP
$C_{100}(5,5)$/6-31G	Dipole moment	X	–0.18	–0.10	0.00	–0.12	–0.01	–0.07	–0.01	0.07	0.05	0.13
		Y	–0.13	–0.09	–0.06	–0.05	–0.18	–0.09	–0.08	–0.06	–0.21	0.14
		Z	0.25	0.00	–0.03	–0.00	–0.03	0.01	–0.01	–0.01	–0.02	0.01
	Quadrupole moment	XX	–309.11	–316.21	–232.70	–236.37	–153.28	–152.38	–248.16	–248.58	–326.81	–340.67
		YY	–309.10	–305.10	–296.37	–297.59	–287.64	–288.24	–303.37	–304.14	–314.31	–316.01
		ZZ	–334.08	–323.66	–296.34	–297.50	–287.60	–288.20	–303.24	–304.07	–314.31	–315.89
		XY	–13.97	–9.29	–0.01	–0.09	–0.03	0.15	–0.09	–0.01	0.01	0.87
		XZ	22.68	19.42	0.01	–0.27	0.011	0.05	0.07	0.17	0.02	0.20
		YZ	17.75	10.91	–0.07	–0.01	–0.01	0.00	–0.02	0.02	–0.00	0.06
	Octapole moment	XXX	–2.48	–4.60	0.03	–1.89	–0.08	–1.71	0.10	2.01	1.120	2.79
		YYY	–1.47	–2.09	–0.43	–0.43	–0.11	0.21	–0.44	0.47	2.75	4.46
		ZZZ	6.07	–3.51	–0.22	–0.11	–0.03	0.09	–0.01	0.12	0.15	0.2439
		XYY	–1.39	–2.09	0.08	–0.25	–0.33	–0.30	1.61	0.27	–1.50	–4.31
		XXY	–1.52	–2.56	–1.10	–1.50	–1.53	–0.57	–1.47	–1.74	2.84	5.51
		XXZ	2.62	1.80	–0.62	0.12	–0.31	0.48	–0.01	–0.31	0.10	0.49
		XZZ	–3.64	0.63	–0.07	–0.32	0.30	–0.05	–1.64	0.13	1.77	5.28
		YZZ	–2.30	–0.06	–0.14	–0.13	–0.04	0.07	–0.17	0.12	0.88	1.37
		YYZ	1.54	1.34	–0.07	–0.05	–0.01	0.07	0.10	0.14	0.11	0.10
		XYZ	1.59	1.28	–0.07	–0.14	0.11	0.01	–1.02	0.27	–0.30	–1.06
	Hexa-decapole moment	XXXX	–12378.34	–12711.56	–20184.34	–20570.90	–17699.00	–17945.43	–20421.61	–20663.78	–22832.84	–23556.02
		YYYY	–6742.94	–6661.57	–4014.70	–4023.31	–3964.90	–3969.93	–4040.41	–4046.09	–4096.83	–4106.79
		ZZZZ	–12970.51	–12592.19	–4014.30	–4022.48	–3963.71	–3968.66	–4037.42	–4045.04	–4094.32	–4101.93
		XXXY	–2509.35	–2468.83	–0.27	–2.61	–0.13	5.49	–4.92	0.67	–3.52	26.90
		XXXZ	4282.84	4381.02	0.59	–8.29	–0.10	1.28	4.09	5.54	0.64	5.41
		YYYX	–2454.27	–2374.62	–2.17	–5.00	12.02	17.85	7.58	9.04	–2.42	4.24
		YYYZ	2409.24	2330.17	–0.02	–0.07	–0.04	–0.00	–0.59	0.06	–0.04	0.37
		ZZZX	4656.95	4491.40	–1.80	–5.38	1.99	2.79	2.34	5.77	0.87	1.25
		ZZZY	2629.38	2488.45	0.01	–0.00	–0.03	–0.01	0.27	–0.01	–0.07	–0.02
		XXYY	–3338.64	–3262.92	–4226.41	–4261.43	–3989.93	–4009.88	–4265.15	–4289.05	–4488.98	–4549.19
		XXZZ	–4427.96	–4401.22	–4225.80	–4259.16	–3989.63	–4009.64	–4263.75	–4289.46	–4491.23	–4548.65
		YYZZ	–3294.19	–3222.93	–1338.17	–1341.01	–1321.45	–1323.15	–1346.63	–1348.57	–1365.37	–1368.42
		XXYZ	975.08	906.32	–0.11	–0.31	–0.10	0.21	0.21	0.68	0.18	2.60
		YYXZ	1530.64	1456.35	1.87	3.88	–1.70	–2.52	–3.33	–4.91	–0.98	0.50
		ZZXY	–1033.40	–944.64	2.10	4.52	–12.17	–17.04	–6.146	–9.15	2.01	1.421

Table 3. Continuation

			$SWCNT_{100}$		$SWCNT_{100}$-Na		$SWCNT_{100}$-Mg		$SWCNT_{100}$-Al		$SWCNT_{100}$-Si	
			HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP
C_{100}(5,5)/6-31G*	Dipole moment	X	–0.03	0.02	0.00	–0.24	0.00	–0.32	0.00	0.07	0.04	0.53
		Y	–0.02	–0.08	–0.06	0.08	–0.09	0.11	0.02	0.01	–0.27	–0.07
		Z	0.10	–0.13	–0.03	0.14	–0.02	–0.11	0.01	0.01	–0.02	–0.03
	Quadrupole moment	XX	–364.48	–360.29	–298.58	–289.96	–210.69	–195.67	–311.51	–300.29	–398.16	–396.51
		YY	–359.91	–338.61	–340.21	–324.81	–325.47	–309.74	–346.25	–330.32	–363.78	–347.81
		ZZ	–393.96	–368.31	–340.20	–325.02	–325.41	–309.99	–346.17	–330.28	–364.02	–348.10
		XY	–20.37	–15.20	0.02	0.51	0.01	0.85	0.03	–0.02	0.05	–0.08
		XZ	33.39	32. 60	–0.01	0.45	–0.01	0.23	–0.05	–0.01	0.00	0.00
		YZ	24.67	17.35	–0.012	0.05	–0.02	0.19	–0.04	0.01	0.01	0.01
	Octapole moment	XXX	0.73	–2.11	0.21	–7.69	–0.06	–11.22	0.02	2.72	0.99	18.16
		YYY	0.42	–2.43	–0.48	0.30	–0.32	0.80	0.09	0.33	–0.40	1.69
		ZZZ	4.35	–6.36	–0.24	0.62	–0.08	–0.36	–0.08	0.15	–0.07	0.01
		XYY	0.39	–2.25	–0.05	–1.22	–0.70	–1.53	0.24	0.01	0.31	–2.03
		XXY	0.36	–2.34	–3.81	–3.73	–2.53	–0.62	–0.06	–1.71	–0.87	–3.31
		XXZ	0.40	0.47	–1.90	–0.34	–0.51	–4.43	–0.02	–0.04	–0.10	–0.82
		XZZ	–1.90	2.06	0.07	–0.36	0.69	–0.39	–0.23	0.36	–0.03	4.92
		YZZ	–1.01	0.61	–0.15	0.06	–0.10	0.31	–0.02	0.10	–0.24	0.47
		YYZ	–0.01	1.19	–0.06	0.15	–0.03	–0.18	0.10	0.03	–0.00	0.03
		XYZ	0.16	1.03	0.22	–0.63	0.24	0.25	–0.217	0.08	0.01	–0.66
	Hexa-decapole moment	XXXX	–14834.71	–14665.30	–25227.68	–24493.30	–22194.41	–21268.98	–25418.45	–24567.72	–28378.87	–27853.34
		YYYY	–8046.42	–7553.66	–4735.76	–4500.00	–4616.05	–4379.37	–4749.88	–4511.32	–4886.25	–4641.52
		ZZZZ	–15636.48	–14554.55	–4735.32	–4500.93	–4614.55	–4379.90	–4748.56	–4510.42	–4887.80	–4641.57
		XXXY	–3051.03	–2893.54	0.63	24.36	0.58	29.79	0.72	–0.52	–1.72	–3.03
		XXXZ	5237.31	5201.33	–0.20	25.86	–0.53	2.95	–1.39	–1.14	–0.44	0.07
		YYYX	–2961.68	–2731.18	18.12	7.88	–11.92	10.14	–18.60	–2.97	–33.06	–16.91
		YYYZ	2894.67	2677.93	–0.07	0.37	–0.06	0.86	–0.17	0.14	–0.05	–0.04
		ZZZX	5693.30	5320.90	15.79	7.04	–1.90	1.71	–9.10	–1.33	8.05	4.01
		ZZZY	3219.91	2940.81	–0.05	–0.07	–0.06	0.25	–0.15	–0.02	0.30	0.09
		XXYY	–4007.46	–3741.48	–5033.51	–4816.71	–4704.85	–4471.26	–5063.70	–4844.82	–5375.80	–5178.34
		XXZZ	–5403.63	–5192.82	–5033.54	–4825.20	–4704.32	–4480.998	–5062.13	–4844.24	–5383.13	–5192.62
		YYZZ	–3955.63	–3700.74	–1578.50	–1500.41	–1538.44	–1459.89	–1583.10	–1503.69	–1628.37	1546.99
		XXYZ	1250.46	1129.04	–0.130	4.87	–0.17	5.98	–0.61	0.85	0.48	0.83
		YYXZ	1867.13	1708.50	–15.88	–3.44	1.91	–0.70	8.58	1.62	–8.22	–4.14
		ZZXY	–1320.54	–1175.41	–18.02	–4.57	11.96	–5.23	18.94	3.25	31.60	15.49

Table 3. Continuation

			$SWCNT_{100}$		$SWCNT_{100}$-Na		$SWCNT_{100}$-Mg		$SWCNT_{100}$-Al		$SWCNT_{100}$-Si	
			HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP
C_{120}(6/6/6)-31G	Dipole moment	X	0.00	–6.30	0.00	–0.33	0.01	–0.04	0.03	0.01	12.81	0.75
		Y	0.00	–0.14	–0.25	–0.23	–0.54	–0.37	–0.55	–0.41	–1.58	–0.59
		Z	0.00	–0.02	–0.02	–0.10	–0.04	–0.03	–0.02	–0.02	0.00	–0.02
	Quadrupole moment	XX	–399.61	–448.21	–331.86	–329.80	–257.61	–248.96	–334.13	–331.64	–489.64	–454.37
		YY	–398.56	–399.39	–393.25	–394.55	–378.72	–377.62	–395.11	–396.14	–416.45	–416.77
		ZZ	–398.56	–398.75	–393.25	–394.94	–378.80	–377.90	–395.24	–396.17	–416.68	–420.21
		XY	–0.02	–0.86	0.02	–0.07	0.02	0.09	0.00	–0.04	5.63	0.00
		XZ	0.00	0.42	–0.01	0.02	–0.01	0.01	0.00	0.02	–0.16	0.00
		YZ	0.00	–0.28	0.01	0.03	0.01	0.01	0.03	0.00	0.04	–0.24
	Octapole moment	XXX	–0.06	–208.20	0.07	–10.14	0.17	–2.07	0.83	0.36	575.16	22.44
		YYY	–0.02	–0.89	–1.04	–1.12	–1.04	–0.31	0.58	0.63	–5.78	–1.72
		ZZZ	0.00	–0.14	–0.07	–0.64	–0.08	–0.03	0.06	–0.02	–0.57	–0.11
		XYY	–0.01	–24.02	0.01	–1.57	0.01	–0.77	0.02	0.30	45.56	1.59
		XXY	–0.06	–3.95	–1.22	–2.29	–1.08	–1.16	–1.91	–1.30	–28.48	2.54
		XXZ	–0.02	–0.63	–0.12	–2.63	–0.13	–0.20	–0.09	–0.17	1.10	–0.03
		XZZ	–0.02	–28.01	0.01	–1.28	0.03	0.38	0.19	–0.21	44.89	4.86
		YZZ	0.00	–0.32	–0.35	–0.36	–0.35	–0.02	0.18	0.22	–2.17	0.01
		YYZ	0.00	–0.05	–0.03	–0.17	–0.03	–0.02	–0.03	0.02	0.70	0.10
		XYZ	0.01	–1.48	0.06	–0.36	0.00	–0.15	–0.10	–0.15	–0.10	–8.80
	Hexa-decapole moment	XXXX	–29701.68	–32328.79	–27409.27	–27450.98	–25090.08	–24951.67	–27404.65	–27437.45	–33078.50	–31471.99
		YYYY	–9251.81	–9239.73	–9162.34	–9182.31	–9032.19	–9033.41	–9161.62	–9179.95	–9289.85	–9310.47
		ZZZZ	–9251.55	–9233.44	–9160.87	–9184.35	–9030.99	–9033.88	–9159.11	–9176.85	–9287.31	–9355.66
		XXXY	–0.67	–27.41	0.63	–2.246	0.56	2.77	–0.31	–1.25	193.91	0.73
		XXXZ	–0.10	13.38	–0.22	0.48	–0.49	0.09	–0.12	0.47	–7.27	2.20
		YYYX	–0.13	–5.96	0.17	1.13	–1.85	–0.421	0.95	0.19	34.61	–0.18
		YYYZ	–0.01	–0.23	0.02	0.03	0.04	0.04	0.09	–0.02	–2.99	–1.48
		ZZZX	–0.01	2.95	0.94	–0.22	0.39	0.34	2.31	1.72	8.36	1.35
		ZZZY	0.02	–2.44	0.01	0.23	0.01	0.01	0.05	–0.09	3.06	–2.54
		XXYY	–6538.44	–6736.73	–6196.05	–6221.90	–5842.05	–5837.07	–6193.70	–6225.32	–6824.34	–6689.60
		XXZZ	–6538.41	–6714.49	–6195.09	–6231.99	–5841.76	–5843.52	–6193.14	–6221.34	–6817.42	–6792.91
		YYZZ	–3083.89	–3080.68	–3053.87	–3061.14	–3010.53	–3011.14	–3053.45	–3059.50	–3094.67	–3110.29
		XXYZ	0.02	–12.07	0.00	1.69	0.04	0.14	0.60	0.00	–0.54	–8.04
		YYXZ	–0.04	0.72	–0.95	0.39	–0.46	–0.26	–2.23	–1.53	–9.40	0.65
		ZZXY	–0.00	–1.53	–0.04	–1.77	1.99	1.16	–0.55	–0.59	16.08	0.60

Table 3. Termination

			$SWCNT_{100}$		$SWCNT_{100}$-Na		$SWCNT_{100}$-Mg		$SWCNT_{100}$-Al		$SWCNT_{100}$-Si	
			HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP	HF	B3LYP
C_{120}(6,6)/6-31G*	Dipole moment	X	0.57	–14.89	2.81	–13.89	0.45	13.53	0.92	–13.01	–0.08	0.05
		Y	–0.01	0.03	–0.06	0.09	–0.15	–0.04	–0.28	–0.26	–0.56	–0.69
		Z	0.01	–0.01	0.00	0.04	0.14	0.03	0.01	–0.01	0.02	–0.03
	Quadrupole moment	XX	–531.37	–563.37	–448.86	–484.84	–343.08	–401.44	–451.44	–486.01	–562.16	–660.68
		YY	–437.93	–456.10	–423.37	–442.09	–399.67	–421.07	–425.51	–444.66	–454.59	–473.33
		ZZ	–437.95	–456.11	–423.26	–441.95	–400.09	–421.19	–425.43	–445.10	–454.41	–474.19
		XY	–0.09	0.14	–1.18	0.84	–0.17	–1.35	–0.17	0.55	0.17	–0.08
		XZ	–0.02	–0.06	0.48	0.22	–0.27	–0.22	–0.22	0.04	0.19	–0.11
		YZ	–0.02	–0.01	0.08	–0.08	0.36	0.09	–0.01	0.11	–0.04	0.12
	Octapole moment	XXX	18.94	–685.49	90.10	–661.66	13.68	657.88	30.58	–639.82	–2.45	1.55
		YYY	–0.06	0.17	0.15	0.74	1.38	1.10	1.38	1.84	–1.50	–1.39
		ZZZ	0.08	–0.08	0.34	0.12	1.08	0.35	0.35	–0.23	0.64	–0.08
		XYY	2.40	–55.35	11.83	–50.81	8.86	48.24	1.72	–44.66	–9.17	1.06
		XXY	–0.34	0.80	0.77	4.63	3.94	8.84	–0.22	3.94	2.01	11.04
		XXZ	0.52	–0.31	0.06	1.32	4.41	1.30	0.86	0.29	–2.21	0.21
		XZZ	2.44	–55.38	11.52	–49.72	–5.00	49.00	4.16	–47.28	8.51	–0.67
		YZZ	–0.03	0.06	–0.14	0.25	0.03	0.65	0.38	0.73	–0.63	–0.44
		YYZ	0.03	–0.02	–0.30	0.28	0.39	0.06	–0.01	0.40	–0.22	–0.03
		XYZ	–0.01	–0.04	0.01	–0.52	–4.39	0.04	–1.18	0.91	8.87	0.34
	Hexa-decapole moment	XXXX	–38390.48	–40719.22	–35421.11	–37852.06	–31675.14	–34971.92	–35405.18	–37776.64	–38921.22	–44494.04
		YYYY	–10270.91	–10755.18	–10048.77	–10520.79	–9791.81	–10283.64	–10047.24	–10530.07	–10330.34	–10741.30
		ZZZZ	–10270.79	–10755.00	–10045.64	–10517.67	–9791.55	–10282.62	–10042.52	–10531.31	–10319.32	–10746.63
		XXXY	–2.79	4.86	–37.38	28.32	–4.86	–42.18	–5.77	18.69	5.45	–3.00
		XXXZ	–0.80	–2.10	15.05	7.12	–8.15	–6.53	–6.99	1.34	6.94	–3.70
		YYYX	–0.63	0.88	–7.49	5.42	–1.93	–11.10	–0.76	4.37	0.15	–2.07
		YYYZ	–0.98	–4.92	0.54	14.64	3.45	–3.56	0.35	14.93	1.08	0.60
		ZZZX	–0.62	–0.36	1.01	2.07	–1.91	–1.01	0.00	2.63	3.66	2.98
		ZZZY	0.80	4.86	0.21	–15.36	–1.19	3.89	–0.49	–14.08	2.26	0.61
		XXYY	–7667.54	–8024.07	–7169.92	–7546.97	–6593.21	–7069.99	–7173.16	–7525.41	–7756.63	–8302.39
		XXZZ	–7667.48	–8024.15	–7167.41	–7541.35	–6622.38	–7073.03	–7160.33	–7541.94	–7757.57	–8321.83
		YYZZ	–3423.79	–3566.48	–3348.04	–3504.16	–3263.29	–3410.87	–3349.49	–3503.99	–3442.64	–3581.37
		XXYZ	–0.49	–0.35	3.45	–3.51	22.34	1.32	–0.68	7.46	–21.20	5.14
		YYXZ	0.38	–0.22	3.28	–0.08	–0.38	–0.84	–1.90	–2.26	–2.40	–3.95
		ZZXY	–0.16	0.43	–2.86	1.82	0.51	–0.70	–0.80	0.46	1.54	1.36

In fact, it was determined that SWCNT blocked potassium channels in a dose-dependent manner. Fullerenes were discovered to be less effective channel blockers than CNT. The mechanism was solely dependent on the size and shape of the nano-particles. They also concluded that electrochemical interactions are between CNT and the ion channels.

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