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Incapsulation of "armchair "-type nanotubes by the Fe atoms chains

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Structural, electronic and magnetic properties of " armchair " nanotubes (NT), incapsulated by the chain of Fe atoms have been investigated. Electronic and magnetic properties have been calculated within the density functional theory and pseudopotential method (package VASP [1]).

We have considered the three options for encapsulating the NT of Fe atoms: 1) one Fe atom per NT unit cell; 2) 1.5 Fe atoms per NT unit cell; 3) 2 Fe atoms per NT unit cell. The results of self-consistent calculations are shown in the table.

Table. Structural parameters, electronic and magnetic properties of "armchair" NT, encapsulated by the chain of Fe atoms.

(n,n)	V	N_C	N_{Fe}	R	m_1	m_2	m_3	U_1	U_2	U_3	E_b
(4,4)	1	32	2	2,78	2,75	2,75		0,61	0,61		+0,248
	2	32	3	2,28	-2,24	-1,46	0,81	0.968	1,016	0,982	+0,289
	3	16	2	2,78	-0,15	2,17		1,101	0,892		+0,333
(5,5)	1	40	2	3,44	3,16	3,16		0,25	0,25		+0,081
	2	40	3	3,44	2,81	2,63	3,10	0,989	1,267	0,03	-0,194
	3	20	2	3,44	2,63	2,63		1,07	1,07		-0,057
(6,6)	1	48	2	4,12	3,09	3,10		0,016	0,018		-0,027
	2	48	3	4,12	3,01	2,62	2,85	0.262	1.820	0.358	-0,156
	3	24	2	4,12	2,87	2,87		0,945	0,945		+0,029
(7,7)	1	56	2	4,79	3.08	3.09		0.005	0.005		-0.037
	2	56	3	4,79	2.99	3.01	2.98	0.775	1.133	0.800	-0.017
	3	28	2	4,79	2,87	2,87		0,947	0,947		-0,021
(8,8)	1	64	2	5,47	3.08	3.08		0.0	0.0		-0.027
	2	64	3	5,47	2.977	2.98	2.87	0.818	1.077	0.820	-0.024
	3	32	2	5,47	2.87	2.87		0.951	0.951		-0.021

Note: N_C, N_{Fe} - the number of carbon and iron atoms in the cell; R - average optimized radius of NT, encapsulated by the iron chain, Å; m_i – magnetic moment per atom of Fe (i), $\mu_Б$; U_i - deviation of Fe (i) atom from NT axis, Å; E_b - the binding energy per atom of the metal, eV.

1. *Kresse G., Hafner J.* Ab initio molecular dynamics for open-shell transition metals // Phys. Rev. B.- 1993.- 48.- P.13115-1 -13115-4.