Supplementary Information

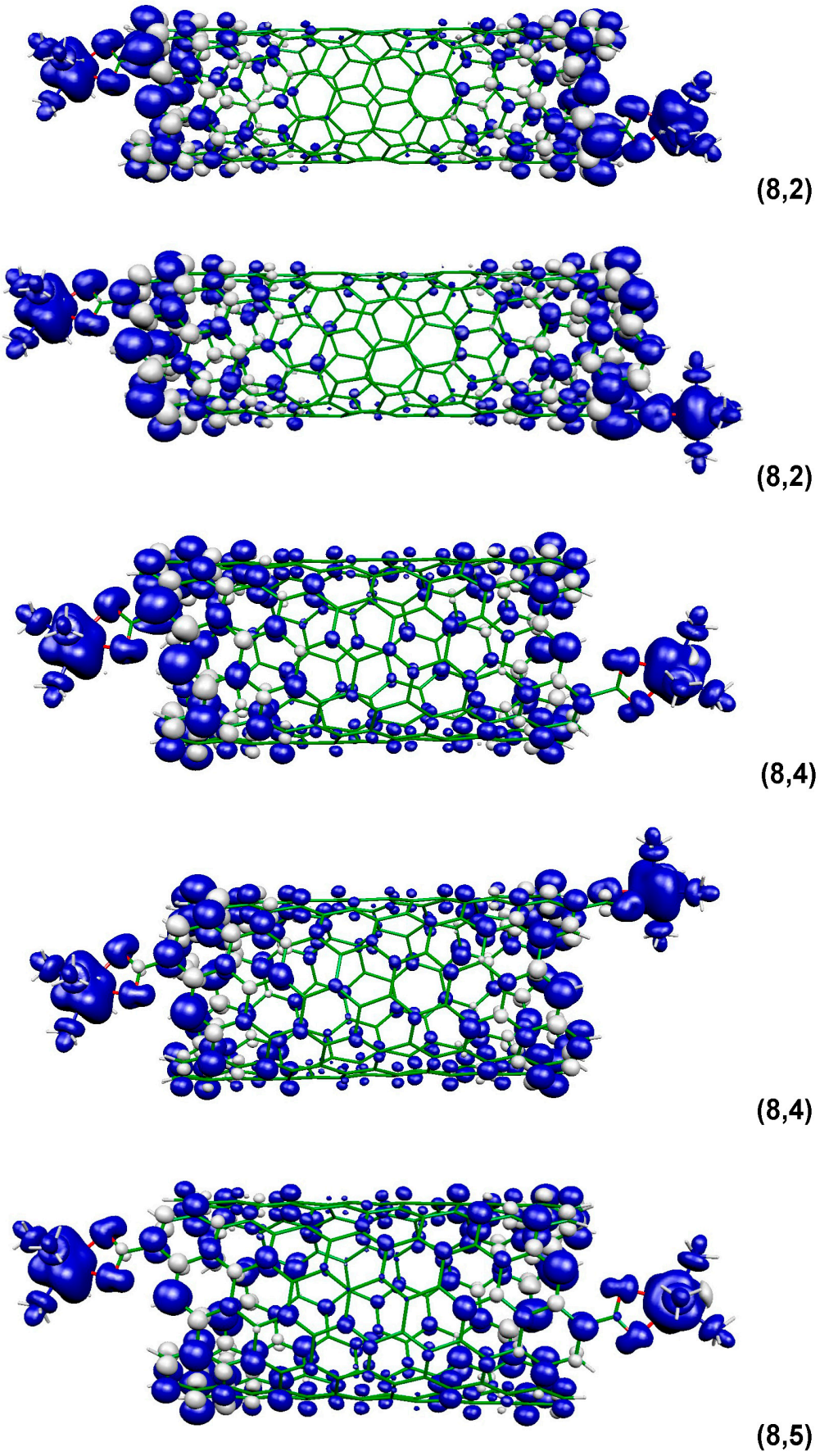

Figure S1. *Cont.*

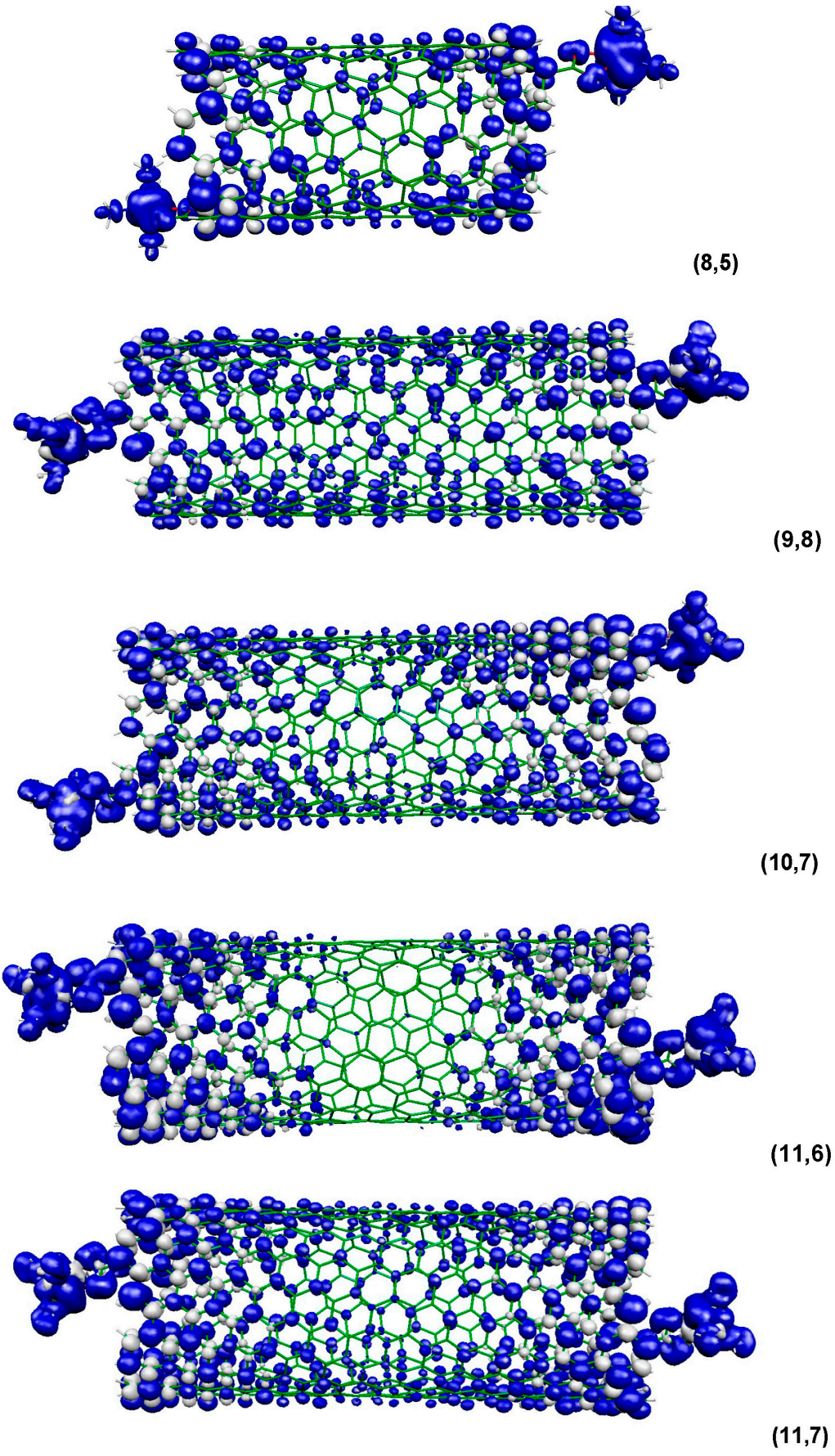

Figure S1. *Cont.*

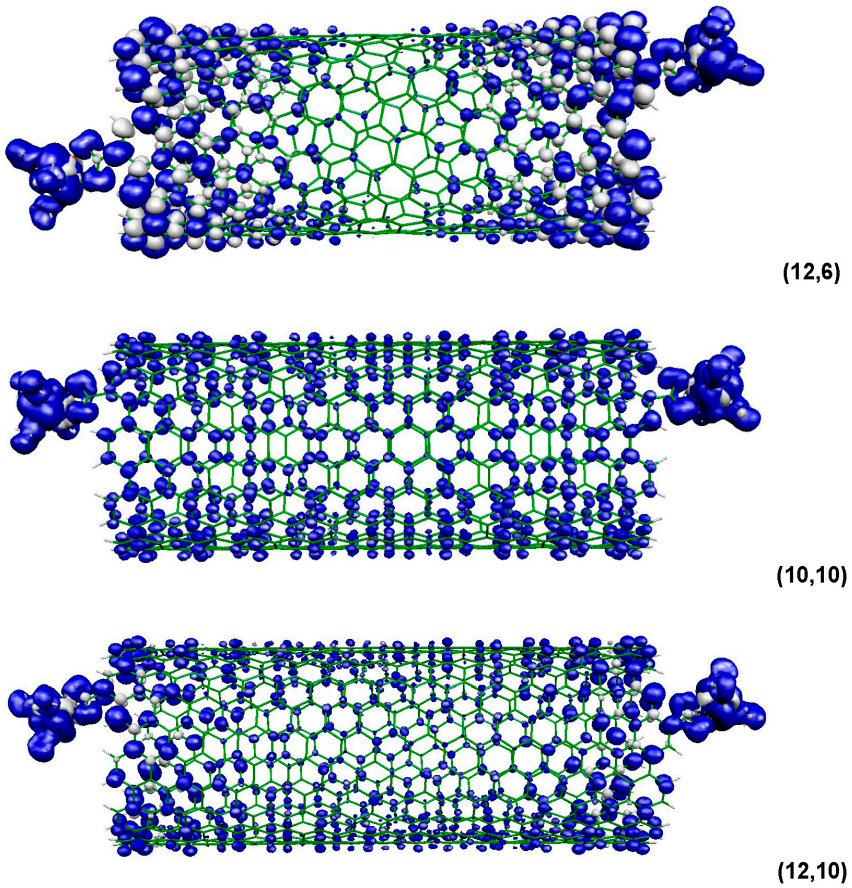

Figure S1. Representation of the spin distributions for the ferromagnetic solution of some Fe^{III} metal-complex SWNT (see Table 1 for the calculated J values). Dark and clear regions indicate positive and negative spin populations, respectively. The isodensity surfaces represented for the ten cases correspond to a value of 0.001 e^{-}/bohr^3.

Optimized Structure

The (7,6) nanotube has been optimized. The ferromagnetic solution has been optimized and this geometry has been employed for the calculation of both ferro and antiferromagnetic spin distributions. There are not important qualitative changes in the calculated J values when the structures are optimized. The exchange coupling constant varies slightly, from +17.2 cm^{-1} for the model structure to +13.4 cm^{-1} for the optimized structure.

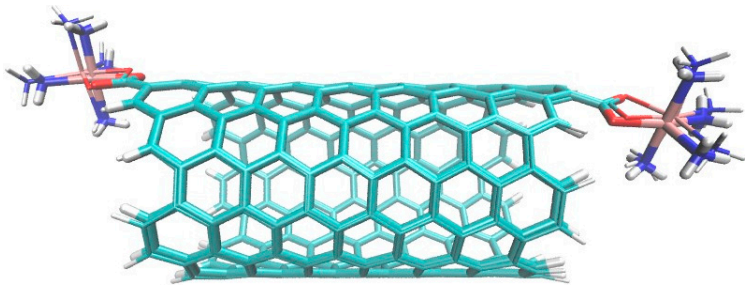

Figure S2. Superposition of the model structure (bold stick) and the optimized structure (small stick) for the (7,6) nanotube.

Table S1. Shift of C_{60} molecules inside (11,6) and (9,8) nanotubes.

Chirality	Transport	Diameter	Shift C_{60}	J_{calc}
(9,8)	SC	11.53	0	+18.2
			−0.2	+16.5
			0.2	+17.4
			0.4	+17.4
(11,6)	SC	11.69	0	−4.1
			0.2	−4.5
			0.4	−4.7
			0.8	−5.0