

Table 1. Physicochemical parameters of group VIII metals determining their reactivity with carbon nanotubes under the electron beam.

Metal	Cohesive energy ^[32] [kJ mol ⁻¹]	M–C σ -bond energy ^{a)} [kJ mol ⁻¹]	M–C π -bond energy ^{b)} [kJ mol ⁻¹]	Stable carbide ^[33]
Os	1713	1040	84	No
Ru	1142	898	160	No
Fe	898	802	90	Yes

^{a)}Calculated for σ -bonding of corresponding metal atoms with a tetra-vacancy defect in a SWNT sidewall; binding energies for mono- and di-vacancy follow the same trend of relative energies;

^{b)}Calculated for the concave side of a carbon nanotube.