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Supporting Information

Theoretical investigation on carbon nucleation on nickel carbides at initial stages of single-walled carbon nanotube formations

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Table S1. Geometric structure parameters of the optimized $Ni_{55}C_n$ (n=5, 10, 15, and 20). As sketched in Fig. 3, the □$_4$, □$_5$, and □$_6$ denote the C atoms coordinated with four, five, or six Ni atoms, respectively. All values of the Ni-Ni bond length (R_{Ni-Ni}), the Ni-C bond length (R_{Ni-C}), the C-C bond length (R_{C-C}) are given in angstrom (Å).

Cluster	R_{Ni-Ni}	R_{Ni-C}	R_{C-C}	□$_4$	□$_5$	□$_6$
$Ni_{55}C_{5a}$	2.29, 2.30, 2.56, 2.62, 2.63, 2.65, 2.88, 2.90, 2.91, 2.98, 2.99, 3.03, 3.07, 3.23, 3.24, 3.28	1.76, 1.78, 1.85, 1.94, 1.95, 1.98	2.60, 2.75, 2.76, 2.85	-	3	2
$Ni_{55}C_{5b}$	2.41, 2.45, 2.48, 2.50, 2.52, 2.58, 2.81, 2.84	1.81, 1.83, 1.91, 1.94	3.65, 3.67	-	-	5
$Ni_{55}C_{10a}$	2.40, 2.41, 2.42, 2.44, 2.45, 2.46, 2.47, 2.48, 2.50, 2.51, 2.52, 2.53, 2.55, 2.57, 2.63, 2.68, 2.69, 2.90, 2.94, 2.95, 3.20, 3.47, 3.62	1.80, 1.82, 1.83, 1.84, 1.85, 1.89, 1.92, 1.96	3.05, 3.06, 3.35, 3.36, 3.63	5	-	5
$Ni_{55}C_{10b}$	2.32, 2.36, 2.38, 2.39, 2.40, 2.41, 2.42, 2.43, 2.44, 2.45, 2.46, 2.47, 2.48, 2.49, 2.50, 2.51, 2.52, 2.53, 2.54, 2.55, 2.56, 2.57, 2.58, 2.59, 2.61, 2.62, 2.63, 2.64, 2.65, 2.68, 2.69, 2.76, 2.84, 2.86, 3.04, 3.15	1.77, 1.78, 1.80, 1.81, 1.82, 1.83, 1.84, 1.85, 1.86, 1.87, 1.88, 1.90, 1.92, 1.93, 2.04	2.85, 2.93, 3.40, 3.46, 3.47, 3.48, 3.50, 3.51, 3.52, 3.56, 4.46, 4.63, 4.66, 4.68, 4.72, 4.83, 4.84, 5.11, 5.30, 5.59, 5.72	2	7	1

$Ni_{55}C_{10c}$	2.34, 2.36, 2.42, 2.43, 2.44, 2.47, 2.48, 2.50, 2.51, 2.52, 2.54, 2.55, 2.56, 2.59, 2.60, 2.61, 2.69, 2.70, 2.78, 2.84, 3.03	1.80, 1.81, 1.82, 1.86, 1.87, 1.90, 1.93, 1.94, 2.04	3.51, 3.53, 3.64, 4.51	-	5	5
$Ni_{55}C_{10d}$	2.44, 2.45, 2.47, 2.48, 2.49, 2.50, 2.51, 2.52, 2.55, 2.57, 2.58, 2.59, 2.61, 2.63, 2.64, 2.65, 2.66, 3.54, 3.55, 3.56, 3.59, 3.67, 3.68, 3.69	1.81, 1.82, 1.85, 1.86, 1.88, 1.89, 1.91, 1.92, 1.98, 1.99	3.44, 3.45, 3.55, 3.56, 3.57, 3.57, 3.58	3	5	2
$Ni_{55}C_{15a}$	2.32, 2.35, 2.36, 2.39, 2.41, 2.43, 2.44, 2.45, 2.46, 2.47, 2.48, 2.51, 2.52, 2.53, 2.54, 2.55, 2.56, 2.57, 2.58, 2.59, 2.60, 2.61, 2.62, 2.63, 2.66, 2.67, 2.68, 2.69, 2.70, 2.72, 2.73, 2.75, 2.76, 2.77, 2.78, 2.89, 2.99, 3.30, 3.41, 3.43, 3.46, 3.51, 3.52, 3.55, 3.56, 3.61, 3.63, 3.64, 3.68, 3.69, 3.70, 3.71, 3.73, 3.74, 3.75, 3.76, 3.79, 3.82, 3.84	1.75, 1.77, 1.78, 1.79, 1.80, 1.81, 1.82, 1.83, 1.84, 1.87, 1.88, 1.89, 1.90, 1.91, 1.92, 1.94, 1.95, 1.96, 1.99	2.88, 3.09, 3.23, 3.25, 3.29, 3.34, 3.39, 3.44, 3.45, 3.46, 3.47, 3.48, 3.49, 3.50, 3.52, 3.53, 3.54, 3.69, 3.76, 4.36, 4.43, 4.46, 4.49, 4.45, 4.57, 4.58, 4.90, 4.91, 4.92, 4.95	3	9	3
$Ni_{55}C_{15b}$	2.34, 2.37, 2.38, 2.41, 2.42, 2.43, 2.44, 2.45, 2.46, 2.47, 2.49, 2.50, 2.51, 2.52, 2.53, 2.54, 2.55, 2.56, 2.57,2.58, 2.59, 2.61, 2.63, 2.64, 2.65, 2.67, 2.68, 2.69, 2.70, 2.74, 2.78, 3.03, 3.24, 3.29, 3.36, 3.44, 3.52, 3.56, 3.61, 3.62, 3.63, 3.64,	1.78, 1.79, 1.80, 1.81, 1.82, 1.83, 1.84, 1.85, 1.86, 1.87, 1.88, 1.89, 1.90, 1.91, 1.92, 1.93, 1.94, 1.95, 1.96, 1.97, 2.00	2.77, 2.79, 2.94, 2.97, 3.04, 3.31, 3.35, 3.37, 3.41, 3.43, 3.45, 3.47, 3.49, 3.52, 3.53, 3.55, 3.56, 3.58, 3.59, 3.66, 3.84, 4.70, 4.73, 4.74,	2	12	1

$Ni_{55}C_{20}$	3.65, 3.66, 3.67, 3.68, 3.69, 3.71, 3.76, 3.78 2.36, 2.39, 2.40, 2.41, 2.42, 2.43, 2.44, 2.45, 2.46, 2.47, 2.48, 2.49, 2.50, 2.51, 2.52, 2.53, 2.54, 2.55, 2.56, 2.57, 2.59, 2.60, 2.62, 2.63, 2.64, 2.65, 2.66, 2.67, 2.68, 2.70, 2.72, 2.73, 2.74, 2.75, 2.80, 2.93, 2.95, 3.19, 3.30, 3.36, 3.44, 3.45, 3.48, 3.51, 3.53, 3.54, 3.56, 3.57, 3.58, 3.59, 3.61, 3.62, 3.64, 3.66, 3.67, 3.68, 3.70, 3.78, 3.80	1.78, 1.79, 1.80, 1.81, 1.82, 1.83, 1.84, 1.85, 1.86, 1.87, 1.88, 1.89, 1.90, 1.91, 1.92, 1.93, 1.94, 1.95, 1.96, 1.97	4.75, 4.76, 4.78, 4.80, 4.84, 4.86, 4.91 2.85, 2.88, 2.89, 3.02, 3.032, 3.04, 3.08, 3.11, 3.12, 3.18, 3.24, 3.26, 3.28, 3.31, 3.33, 3.36, 3.37, 3.38, 3.40, 3.42, 3.44, 3.52, 3.55, 3.56, 3.58, 3.65, 3.77, 3.86, 4.01, 4.51, 4.58, 4.63, 4.73, 4.78, 4.79, 4.81, 4.82, 4.88, 4.95	9	6	5

Table S2. Adsorption energy E_a (eV) and chemical potential □ (eV) of the carbon rings and caps attached on the $Ni_{55}C_{20}$ carbide or pure Ni_{55} clusters.

System	E_a (eV)	□ (eV)	System	E_a (eV)	□ (eV)
$Ni_{55}C_{20}$Ring5	6.96	1.32	Ni_{55}Ring5	5.91	1.53
$Ni_{55}C_{20}$Ring6	3.05	1.24	Ni_{55}Ring6	5.65	0.81
$Ni_{55}C_{20}$Cap20	5.86	0.58	Ni_{55}Cap20	5.56	0.59
$Ni_{55}C_{20}$Cap21	11.92	0.41	Ni_{55}Cap21	10.15	0.50
$Ni_{55}C_{20}$Cap39	19.24	0.22	Ni_{55}Cap39	20.82	0.22
$Ni_{55}C_{20}$Cap40	11.61	0.24	Ni_{55}Cap40	16.60	0.12