Supplementary Information

Nanocluster Formation and its role in Graphene Chemical Vapor Deposition Growth

SI-1. Various C_{21} isomers on Rh(111)

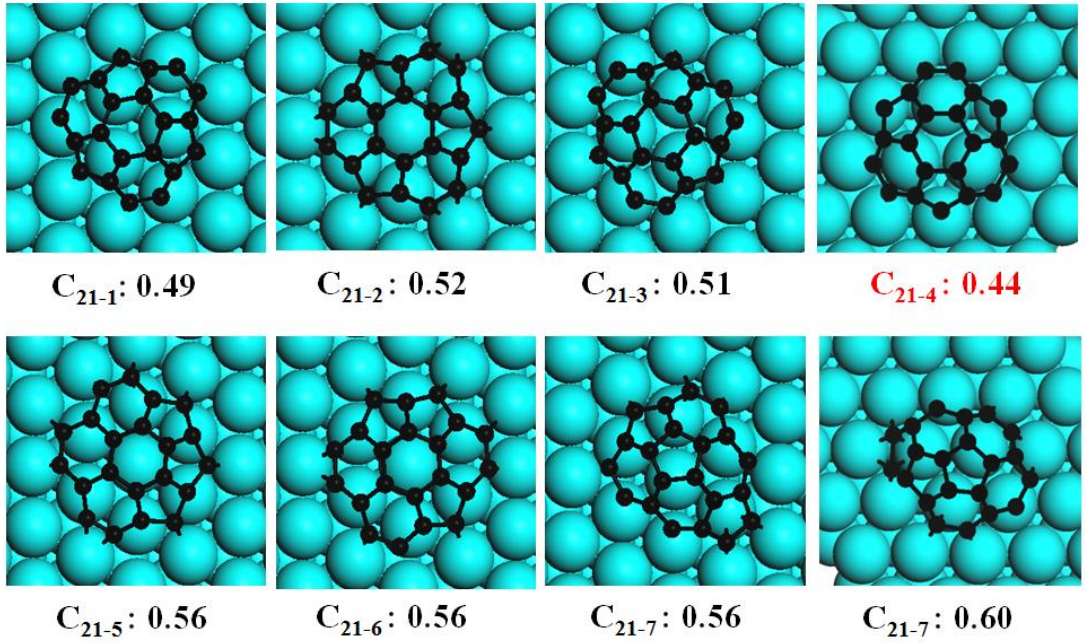

Figure S1. Various isomers of C_{21}@Rh(111) and corresponsing energy (in eV per C atom).

SI-2. Ground structures of C_N (N=16-24) cluster supported by different metal surfaces.

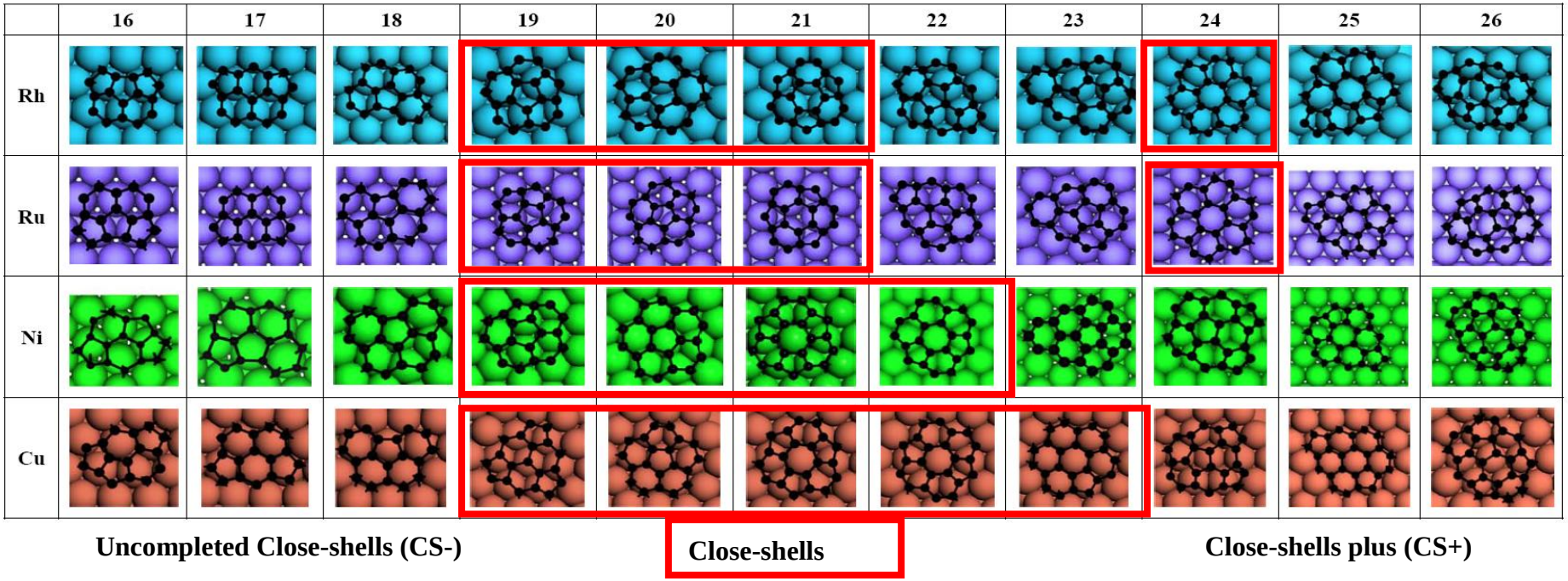

Figure S2. Ground structures of C_N (N=16-24) cluster supported by different metal surfaces. Structures labeled by red rectangle are close-shell structures, left structures are uncompleted close-shell structures and those on the right are close-shell plus one or two rings. Each C_N cluster has several possible network structures and the most stable one was selected as the ground structure.

SI-3. Simulated STM images of C_{21} and C_{24} clusters on Ru(0001), Ni(111) and Cu(111) surfaces.

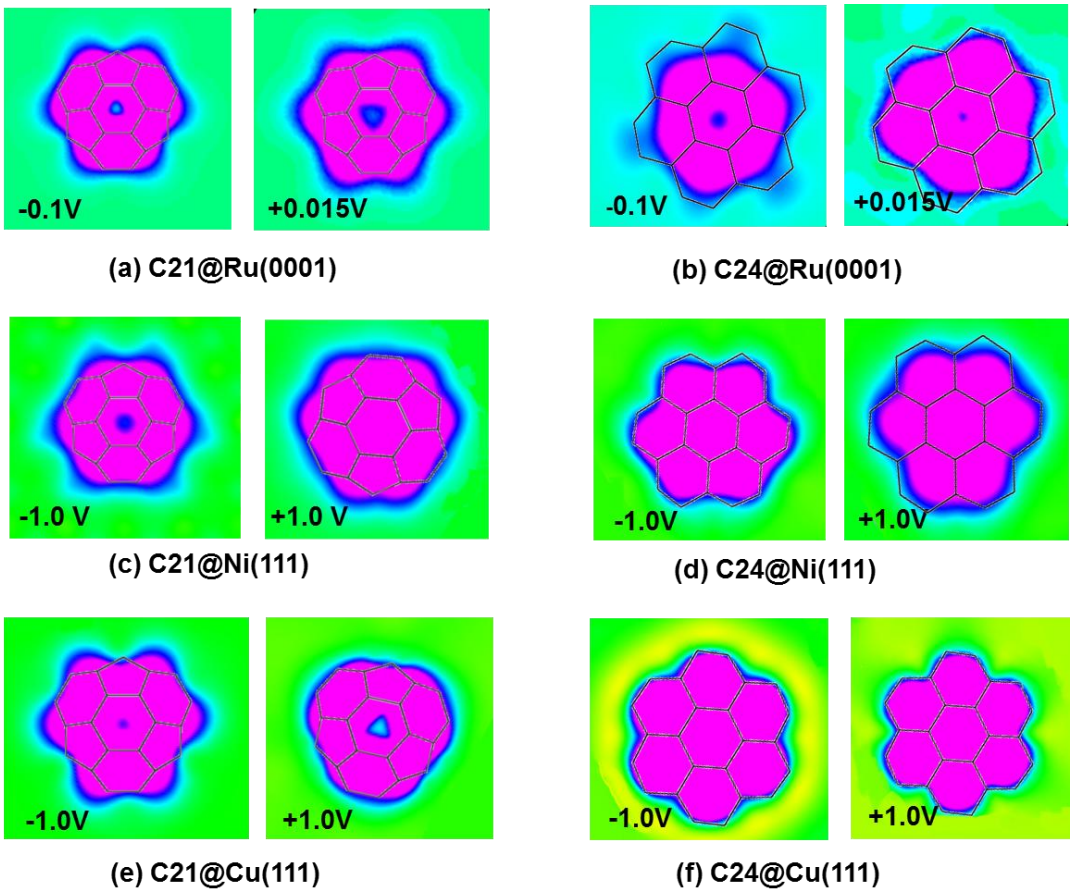

Figure S3. DFT simulated STM images of C_{21} and C_{24} cluster on various metal surface and their atomic structure: (a) C21@Ru(0001) under bias voltage of -0.1V and +0.015 V; (b) C24@Ru(0001) under bias voltage of -0.1V and +0.015 V; (c) C21@Ni(111) under bias voltage of -1.0V and +1.0 V; (d) C24@Ni(111) under bias voltage of -1.0 V and +1.0 V; (e) C21@Cu(111) under bias voltage of -1.0 V and +1.0 V; (f) C24@Cu(111) under bias voltage of -0.1V and +0.015 V.

SI-4. The preference of upright standing graphene nanoribbon

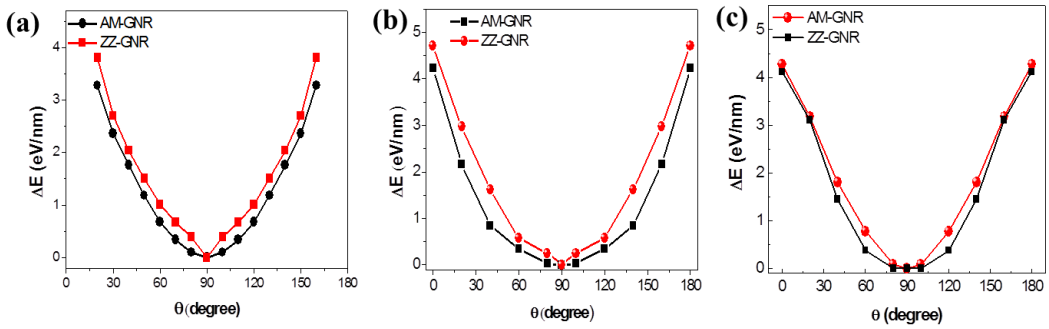

Figure S4. The preference of upright standing zigzag graphene nanoribbon (ZZ-GNR) and armchair graphene nanoribbon (AM-GNR) formation on (a)Ni(111), (b) Ru(0001), and (c) Cu(111) surface.