Supplementary Information for

Formation of carbyne on transition metal surface

Qinghong Yuan[a], Feng Ding[a]*

[a] Institute of Textiles and Clothing, Hong Kong Polytechnic University, Kowloon, Hong Kong, Peoples Republic of China, E-mail: feng.ding@polyu.edu.hk

Computational details

A three layer thick metal slab with the bottom layer fixed was used to represent the metal surfaces (e.g. Cu(111), Ni(111), Rh(111) and Ru(0001)). For each carbon clusters C_N (N=1-17) on metal surfaces, several different configurations are optimized and the lowest one was taken as the ground state structure (see Ref. [1] for details). The super-cell of the slab model is chosen appropriately to avoid the interaction between neighbor carbon clusters. All calculations were carried out using a density-functional theory (DFT) method implemented in the Vienna Ab initio Simulation Package (VASP).[2,3] The ion-electron interactions are treated with the projected augmented wave (PAW) pseudo-potentials[4] and the general gradient approximation (GGA) parameterized by Perdew, Burke and Ernzerhof (PBE)[5] was used as exchange-correlation functional. The kinetic energy cutoff is set as 400 eV. For each structure, energy was optimized until the force component on every atom was less than 0.02eV/Å. Non-spin-polarized DFT methods were used for Cu, Rh and Ru metals and

spin-polarized DFT method was used for Ni. The STM images are obtained for the electron filled states at −2.0 and +2.0 eV bias and calculated within the Tersoff-Hamman approximation.[6]

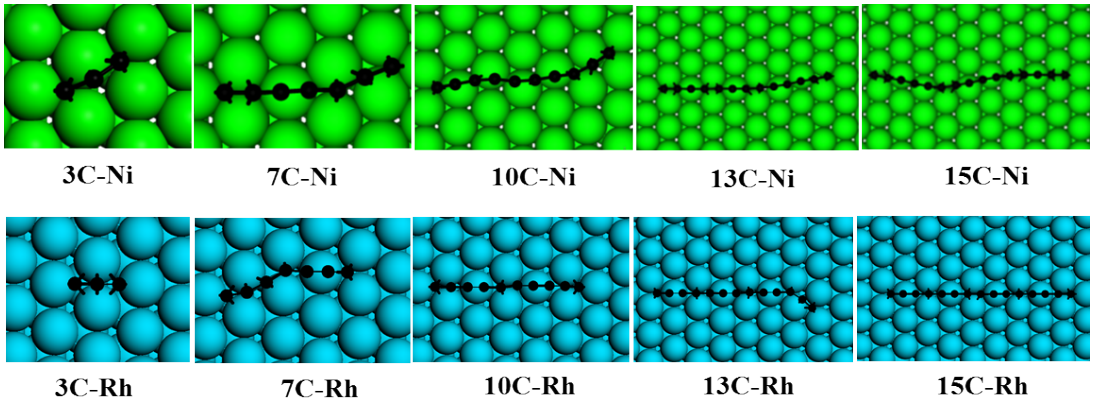

Fig. S1 Selected structures of carbon chains (3C, 7C, 10C, 13C, 15C) on Ni(111) and Rh(111) surfaces.

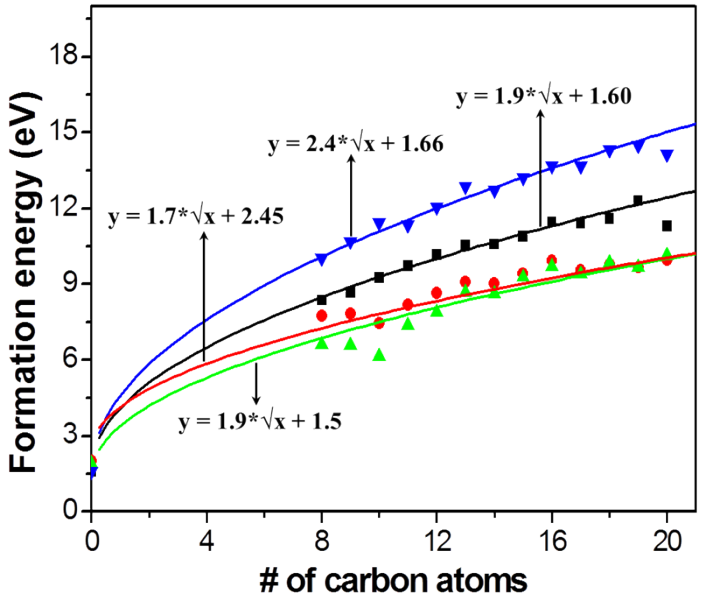

Fig. S2 Formation energies of carbon island consisting of 8–19 atoms on Cu(111), Rh(111), Ru (0001) and Ni(111) surfaces, and the fitting curves for these energies using formula (2).

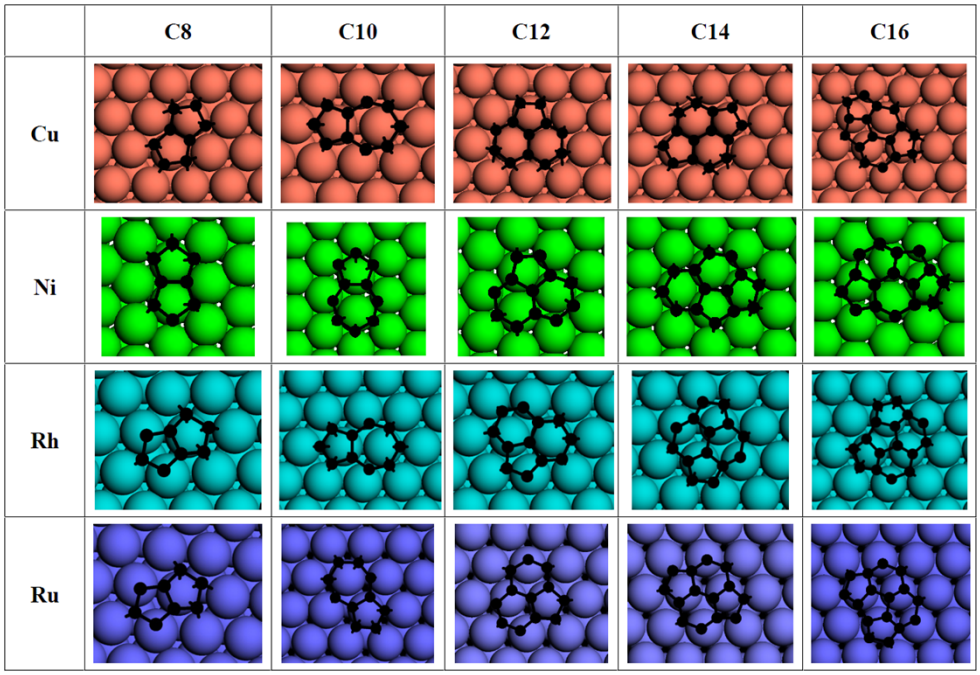

Fig. S3 Selected carbon island structures (8C, 10C, 12C, 14C, 16C) on Cu(111), Ni(111), Rh(111) and Ru(0001) surfaces.

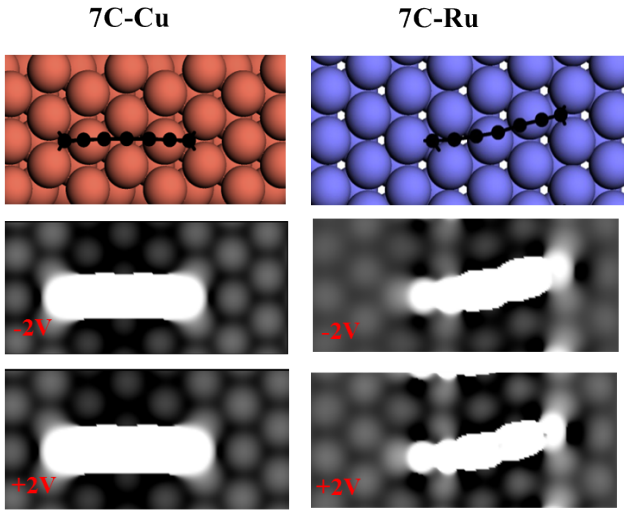

Fig. S4 Simulated STM for carbon chain with 7 carbon atoms on Cu(111) and Ru(0001) surfaces.

References

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