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Graphene nucleation and growth on the transition metal surfaces: the role of pentagon, metal step and magic carbon clusters JUNFENG GAO, JIJUN ZHAO, Dalian University of Technology, FENG DING, Hong Kong Polytechnic University — The nucleation behavior of graphene on transition metal surfaces, either on a terrace or near a step edge, is systematically explored using density functional theory calculations. The supported carbon clusters, CN (N=1∼24), on the Ni(111) surface are carefully optimized [1,2]. A structural transformation from a C chain to a sp^2 C network at C_{12} and the most stable structures of sp^2 graphene islands contain one to three pentagons. In agreement with experimental observations, our calculations show that graphene nucleation near a metal step edge is superior to that on a terrace. Besides, ground state structures of supported CN (N = 16∼26), clusters on four selected transition metal surfaces: (Rh(111), Ru(0001), Ni(111) and Cu(111)) are explored [3]. A core-shell structured of C_{21} stands out as a magic cluster, which is one of the dominating carbon precursors in graphene CVD growth and has been observed in experimental STM images. The energy barrier of two C_{21} clusters' coalescence is computed to illustrate their influence on the kinetics of graphene CVD growth at different temperatures.

[1] J. Gao, et al,. J. Am. Chem. Soc. 133, 5009 (2011).
[2] J. Gao, et al., J. Phys. Chem. C 115, 17695 (2011).
[3] Q. Yuan, et al., J. Am. Chem. Soc. (accepted).

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