Theoretical Investigations of the Mechanisms of Graphene Growth

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Abstract

Massive preparation of high quality graphene is critical for the wide application of graphene. Recently, chemical vapor deposition (CVD) of carbon sources on transition metals surfaces is looked as a promising way, while the growth mechanism of graphene is not clear. Combined density functional (DFT) calculations, molecular dynamics (MD) simulations, thermodynamics analysis, and kinetic Monte Carlo (kMC) simulations, the possible nucleation processes, and the growth kinetics on Cu and Ir surfaces are investigated.

References：

[1] P. Wu, W. H. Zhang, Z. Y. Li, J. L. Yang and J. G. Hou, Coalescence of carbon atoms on Cu(111) surface: Emergence of a stable bridging-metal structure motif, *J. Chem. Phys.* **133**, 071101 (2010).

[2] Z. C. Li, P. Wu, C. X. Wang, X. D. Fan, W. H. Zhan, X. F. Zhai, C. G. Zeng, Z. Y. Li, J. L. Yang, J. G. Hou, Low-Temperature Growth of Graphene by Chemical Vapor Deposition Using Solid and Liquid Carbon Sources, *ACS NANO*, **5**, 3385 (2011).

[3] W. H. Zhang, P. Wu, Z. Y. Li, J. L. Yang, First-Principles Thermodynamics of Graphene Growth on Cu Surfaces, *J. Phys. Chem. C* **115**, 17782 (2011).

[4] P. Wu, H. J. Jiang, W. H. Zhang, Z. Y. Li, Z. H. Hou, J. L. Yang, Lattice Mismatch Induced Nonlinear Growth of Graphene, *J. Am. Chem. Soc.* **134**, 6045(2012).

[5] Z. C. Li, W. H. Zhang, X. D. Fan, P. Wu, C. G. Zeng, Z. Y. Li, X. F. Zhai, J. L. Yang, J. G. Hou, Graphene Thickness Control via Gas-Phase Dynamics in Chemical Vapor Deposition, *J. Phys. Chem. C* **116**, 10557(2012).