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Role of Cooperative Interactions in the Intercalation of Heteroatoms between Graphene and a Metal Substrate SHIXUAN DU, Institute of Physics, Chinese Academy of Sciences — Graphene, a two-dimensional crystal of carbon atoms packed in a honeycomb structure, has many promising mechanical, electrical, and optical properties. The intercalation of heteroatoms between graphene and a metal substrate has been studied intensively over the past few years, due to its effect on the graphene properties, and as a method to create vertical heterostructures. Various intercalation processes have been reported with different combinations of heteroatoms and substrates. In this talk, I will present the investigation of the key processes governing the intercalation of heteroatoms between graphene and a substrate by combining atomic-scale characterization with density functional theory (DFT). Si intercalation between graphene and Ru(0001) is chosen as a test bed. We elucidate the role of cooperative interactions between heteroatoms, graphene, and substrate. By combining scanning tunneling microscopy with density functional theory, the intercalation process is confirmed to consist of four key steps, involving creation of defects, migration of heteroatoms, self-repairing of graphene, and growth of an intercalated monolayer. Other combinations of heteroatoms (such as Ni, Pd and Pt) and substrates (such as Ir(111) and SiC(0001)) are also investigated to support the generality of our study. Both theory and experiments indicate that this mechanism applies also to other combinations of heteroatoms and substrates. (G. Li et al., J. Am. Chem. Soc. 137 (2015) 7099. In collaboration with G. Li, H.T. Zhou, L.D. Pan, Y. Zhang, L. Huang, W.Y. Xu, and H.J. Gao in CAS, Min Ouyang in MU, and A.C. Ferrari in U. Cambridge.)

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