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Theoretical modeling of early stages of graphene growth by epitaxial methods

One method of growing epitaxial graphene is temperature programmed growth (TPG). In this method, hydrocarbon molecules are deposited onto a transition metal surface at room temperature and then the temperature is increased in order to facilitate the thermal decomposition of the hydrocarbons and lead to the formation of graphene flakes. The thermal decomposition mechanism of ethylene was investigated with a combined approach of experimental and theoretical techniques. X-ray photoelectron spectroscopy (XPS) experiments were used along with core level binding energy calculations to identify the evolution of species on the Ir(111) surface as the temperature is increased. A complete reaction scheme incorporating all possible reactions between the various CnHm species, from ethylene to C monomers and dimers, was also developed. The energy barriers for each reaction were calculated using the DFT based nudged elastic band method. For the most important reactions the prefactors to the rates were also calculated. These were then used to simulate the kinetics and determine the species evolution on the surface with time (temperature). This resulting temperature evolution is found to agree with the photoemission measurements. The molecular dissociation mechanism begins with the dehydrogenation of ethylene to vinylidene (CH2C), which is then converted to acetylene (CHCH) by the removal and addition of a H atom. The C-C bond is then broken to form methylidyne (CH), which finally dehydrogenates to produce C monomers that are available for the early stage nucleation of the graphene islands. Our method has laso been applied to Chemical Vapour Deposition (CVD) method and the corresponding resulting mechanism of ethylene and methane decomposition are compared with that obtained using simulations of TPG. Following from this, the nucleation of carbon clusters prior to the formation of graphene islands was also investigated. The number of carbon atoms in the critical cluster, which is equally likely to grow or to shrink in the prevailing conditions, was determined by the considering appropriate nucleation free energy. Using *ab initio* density functional theory calculations, the free energies of carbon clusters (containing up 16 C atoms) on the Ir(111) surface were calculated based on the configurational and vibrational contributions. The results are strongly dependent on temperature, showing its importance to cluster growth. Furthermore, we find that different types of clusters (linear, compact, dome, etc.) are more stable over different size ranges. Then mechanisms, which allow the clusters to reconstruct their structure type, are investigated.

Biography

Lev Kantorovich got his PhD in Latvia (former USSR) in 1985 in the area of Solid State Physics. In 1993-94 he spent one-year in Oviedo, Spain, as an Invited Professor. In 1994, he took a Postdoctoral Position at Keele University (UK), then a number of Postdoctoral appointments followed at University College London since 1996. In 2002, he was appointed a Lecturer at Physics Department of King's College London (UK), then promoted to Reader in 2005 and Professor in 2009. He is a winner of a Teaching Excellence Award (twice: 2005, 2010) and of the Distinguished Supervisor Award (2007). He has been teaching at KCL the second year maths course, and two advanced 4th year sub-courses on Green's functions and group theory. His current research interests lie in modeling STM and AFM imaging of surfaces, as well as imaging and manipulation of atoms and molecules on them; dissipation in non-contact AFM; quantum conductance with non-equilibrium Green's functions (NEGF); classical and quantum Generalised Langevin dynamics; thermostatting in MD simulations; self-assembly of organic molecules on crystal surfaces including kinetics of assemblies; role of van der Waals interaction in surface thermodynamics and interaction of molecules with surfaces; order-N DFT-based methods for extended systems (a fragmentation approach); understanding of growth of graphene by epitaxial methods; kinetics of phase transitions of self-assembled molecular films on surfaces; Kinetic Monte Carlo methods.

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