RCMS Research Center for Materials Science, Nagoya University

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Platform: Nano-Energy

Theoretical Chemistry Colloquium

October 14, 2016 (Fri), 16:00-17:00

RCMS, 2nd floor, Chemistry Gallery

Low dimensional nanomaterials. Theoretical predictions and experimental support

Dr. Dmitry G. Kvashnin
Emanuel Institute of Biochemical Physics Russian Academy of Sciences, Moscow, Russia &
National University of Science and Technology "MISIS", Moscow, Russia

Abstract: Successful synthesis of graphene opens a new field in material sciences - the field of low dimensional materials. Nowadays a high number of scientific groups over the world take many attempts to fabricate and investigate novel two dimensional materials with unexpected physical and chemical properties. This presentation is devoted to the theoretical investigation of low dimensional materials with various compounds. Using classical molecular dynamic calculations the unusual effect of hardening of graphene with the low concentration of vacancy defects was described from atomistic point of view (J. Phys. Chem. Lett., 6, 2384 (2015)). By means of ab initio calculations the physical properties of novel two-dimensional materials based on bilayered graphene and copper oxide were studied in details. All obtained results were confirmed by experimental data (Nano Research 8 (4), 1250 (2015), NanoScale (2016), submitted).

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Contact: Stephan Irle
sirle@chem.nagoya-u.ac.jp, Tel.: 6397