



601st ASRC Seminar

Date: 13:30 ~ 14:30 Friday, 28 August

Location: Meeting Room 103, ASRC bldg.

Speaker: Dr. P.B. Sorokin (National University of Science and Technology MISiS, Technological Institute for Superhard and Novel Carbon Materials)

Title: New specific properties of graphene: ultrahigh stiffness and flexoelectric effect

Abstract: Here I will show that well-known effect of mechanical stiffness degradation under the influence of point defects in macroscopic solids can be controversially reversed in the case of low-dimensional materials. Using atomistic simulation, we showed that a single-layered graphene film can be sufficiently stiffened by monovacancy defects at a tiny concentration. Our results correspond well with recent experimental data and suggest that the effect of mechanical stiffness augmentation is mainly originated from specific bonds distribution in the surrounded monovacancy defects regions. We showed that such unusual mechanical response is the feature of presence of specifically monovacancies [D.G. Kvashnin et al. J. Phys. Chem. Lett. 6 (2015) 2384]. In the second part of the talk, I will be focused on the new effect in graphene electronic properties. It is known that a homogenous mechanical distortion of graphene cannot induce electrical dipole due to graphene lattice central symmetry center. This rule however does not apply to the second order electronic flexoelectric effect induced by the strain gradient, especially by the bending of the graphene sheet. We show that slight variations in atomic structure will lead to significant changes of macroscopic characteristics by the example of dipole moment. Our analysis suggests the possibility of predicting the electric dipole moments of complicated low-dimensional graphene-based systems using only their atomic geometry [A.G. Kvashnin et al. J. Phys. Chem. Lett. 6 (2015) 2740]



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