When: February 28, 16:00-17:00 Where: Skoltech, Blue Bldg, room 402

Computational Materials Science Seminar

MELTING SCENARIOS and UNUSUAL CRYSTAL STRUCTURES in TWO-DIMENSIONAL CORE-SOFTENED SYSTEMS



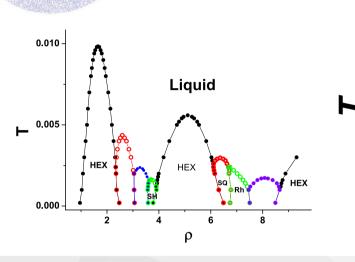
SPEAKER: Valentin. N. Ryzhov

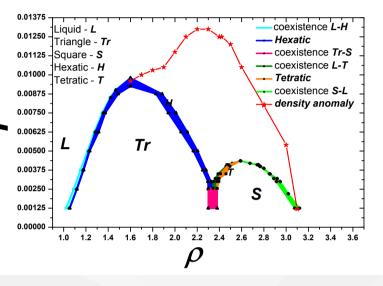
Institute for High Pressure Physics, Russian Academy of Sciences, Troitsk, Moscow, Russia

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ABSTRACT

Recently, there has been growing interest to investigation of behavior of confined fluids, with a special attention to the water. Water plays an important role in many natural processes where it is confined or at contact with substrates, for example, in rocks, in biological cells, at contact with surfaces of proteins, in biological membranes, etc. It is well known, that the qualitative behavior of water, including the water-like anomalies, can be described using the core-softened potentials with two length scales [1,2]. Another example of the core-softened system which also demonstrates complex phase behavior and water-like anomalies is the Hertzian spheres [3,4]. In the talk we present short description of Berezinskii-Kosterlitz-Thouless (BKT) theory, modern melting scenarios of 2D crystals and computer simulation study of phase diagrams of mentioned above 2D systems: core-softened repulsive shoulder potential and Hertzian spheres. It is shown, that in contrast to the case of simple potentials, like soft disks, where the ground state always corresponds to the hexagonal close-packed structure, the various structures are possible including the square, kagome, snub-square lattices and quasicrystalline phase with 12-fold symmetry [5,6]. The possible melting scenarios are discussed and the deviations from the widely accepted Berezinskii-Kosterlitz-Thouless-Halperin-Nelson-Young (BKTHNY) scenario (two BKT transitions with the intermediate hexatic phase) are discussed [5-9]. It is found that depending on the form of the potential, the melting of the systems can occur in accordance with BKTHNY scenario, through one first order transition or through two-stage transition with continuous BKT type solid-hexatic transition and first order hexatic-liquid transition. The influence of the random disorder, which is inevitable in real experiments, on the melting scenario is considered. Random pinning transforms the first order transition into two-stage melting scenario or widens the hexatic phase [7-9]. It gives the possibility to study the behavior of the diffusivity and order parameters in the vicinity of the melting transition and inside the hexatic phase.

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BIOGRAPHY

Valentin Ryzhov was born in Noginsk, Moscow region, in 1952.

Master's degree -1976, Department of Physics, Moscow State University, Russia

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Doctor of Science - 1997, Joint Institute for Nuclear Researches, Dubna. The title of the thesis: "Statistical theory of crystallization of simple systems". From 1976 up to now he is working at the Institute for High Pressure Physics Russian Academy of Sciences: 1976 – post-graduate student, 1997- up to now: Deputy Director. 1997- up to now: Moscow Institute of Physics and Technology (State University), lecturer, 1996-2005 - visiting scientist at Delaware University, 2010 – visiting scientist in Argonne National Laboratory.

Specialization: Condensed Matter Theoretical Physics

Current research interests: Soft Matter, Computer Simulations, Colloids, Polymers, Phase Transitions, Physics of Disordered Systems, Liquids, Glasses, Two-Dimensional Melting, Superconductivity and Bose-Einstein Condensates.

Member of European Physical Society.

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