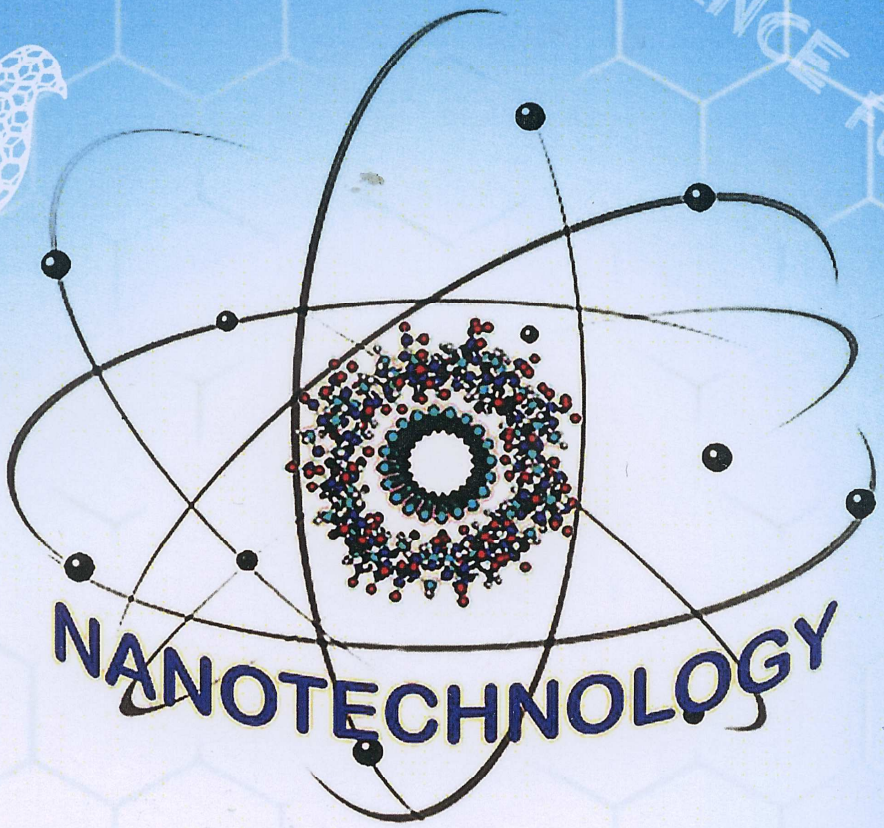

ABSTRACT BOOK

International research and practice conference:

NANOTECHNOLOGY AND NANOMATERIALS (NANO-2017)

23 - 26 August 2017
Chernivtsi
Ukraine

INTERNATIONAL RESEARCH AND PRACTICE CONFERENCE "NANOTECHNOLOGY AND NANOMATERIALS" (NANO-2017)

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BOOK OF ABSTRACTS

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This book contains the abstracts of contributions presented at the International research and practice conference "Nanotechnology and Nanomaterials" (NANO-2017).

The NANO-2017 Conference was organized by the Institute of Physics of NAS of Ukraine with the participation of the Yuriy Fedkovych Chernivtsi National University (Ukraine), University of Tartu (Estonia), University of Turin (Italy), Pierre and Marie Curie University – Paris 6 (France) and Representative office of Polish Academy of Sciences in Kiev.

NANO-2017 was the fifth conference in the series of NANO-conferences initiated by the Institute of Physics of NAS of Ukraine in 2012 in the framework of FP7 Nanotwining project. From year to year, they attract more attention and participants. In 2012, the first meeting was held in the format of International Summer School for young scientists "Nanotechnology: from fundamental research to innovations". The 2013 and 2014 conferences were organized in conjunction with the International Summer Schools for young scientists under the same title. In 2013, this event was attended by more than 300 scientists, in 2014-2015, 450 scientists took part and in 2016 it gathered above 650 participants from Ukraine, Poland, Italy, Estonia, France, Austria, Germany, Greece, Turkey, USA, Romania, Moldova, Czech Republic, Taiwan, Lithuania, Egypt, Iran, India, Algeria, Indonesia and other countries. In 2017 Organizer Committee has received more than 700 application forms from about 25 countries of the world.

The NANO-2017 conference brought together leading scientists and young researchers from many countries of the world. This year its topics were as follows: Nanoobjects' microscopy; Nanocomposites and nanomaterials; Nanostructured surfaces; Nanooptics and photonics; Nanoplasmonics and surface enhanced spectroscopy; Nanochemistry and biotechnology; Nanoscale physics; Physico-chemical nanomaterials science.

This year the NANO-2017 Conference was organized in the framework of the NAS of Ukraine Program «Fundamental issues of creation of new nanomaterials and nanotechnologies» for 2015–2019.

Website of the Nano-2017 conference: http://www.iop.kiev.ua/~nano2017/

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Modelling and first-principles calculation of low frequency quasy-localized vibrations of soft and rigid As-S nanoclusters

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Nowadays the non-crystalline chalcogenides in glassy and thin film forms are important photonic media for both practical usage and fundamental investigations. One of the most intriguing fundamental phenomenon in physics of disordered solids is the excess contribution to the low frequency (LF) vibrational states with respect to the predictions of the Debye theory. This contribution seen as a broad peak in the inelastic (neutron and Raman) scattering intensity around 1 THz. The peak intensity (usually referred to as the Boson peak (BP)) in the 2-10 meV energy range is proportional to the density of states ($g(\omega)$) by the rule of $g(\omega)/\omega^2$ while the Debye theory in this spectral region predicts the constant intensity [1]. The relaxational and vibrational properties of non-crystalline solids in the LF (<100 cm^{-1}) region may contribute to the understanding of anomalous properties at low temperatures, the glass transition and other phenomena observed in disordered materials. While the relaxation dynamics can be described by the mode coupling theory, the vibrational excitations are still unsettled and subject of intense investigation and discussions.

In this work we present the results of modelling of different As-S nanoclusters representing the medium range order structures of As-S glasses and first-principles calculations of low frequency Raman active vibrations. It was established that there is no vibrational contribution from a single AsS3 pyramidal structural units and rigid cage-like As-S nanoclusters. However, the low frequency Raman modes calculated for gas phase medium range order branchy- and ring-like As-S nanoclusters are found to be located in the spectral region of BP observed in the Raman spectra of As-S glasses. Further modelling includes the model of 12-membered ring incorporated in continuous media. The stepwise fixing of the ring in space (by introducing fictive heavy terminal atoms) revealed the localization of the Raman active vibrational modes at extremely low frequency range (2-5 cm^{-1}). It was established that the mode localization and the red-shift of low energy vibrations is depending on degree of freedom of the ring in space.

1 *Holomb R., Mitsa V.* Boson peak of AsxS1-x glasses and theoretical calculations of low frequencies clusters vibrations // Solid State Commun. – 2004. – 129, №10. – P. 655-659.