

*XI International Conference*  
**"Nanotechnology and Nanomaterials"**  
**NANO-2023**

August 16-19, 2023  
Bukovel, Ukraine

*Certificate of attendance*

***Dr. Rabie AMARI***

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*Participated in the conference with the report*

***Electronic and optical properties of of AgXBr<sub>3</sub> (X = Ca and Sr) Perovskites:***

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***An ab initio study with the Tran–Blaha-modified Becke–Johnson density functional***

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Dr. Olena Fesenko  
Head of Local Organizing Committee

**INTERNATIONAL RESEARCH  
AND PRACTICE CONFERENCE  
“NANOTECHNOLOGY  
AND NANOMATERIALS”**

The NANO-2023 Conference is dedicated  
to the brave men and women serving in the Armed Forces  
of Ukraine, who safeguard freedom and peace in Ukraine

**16-19 of August 2023**

**Bukovel, UKRAINE**

**Abstract book**

**УДК 536:669**

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This book contains the abstracts of contributions presented at the International research and practice conference “Nanotechnology and Nanomaterials” (NANO-2023).

The NANO-2023 Conference was organized by the Institute of Physics of NAS of Ukraine with the participation of the University of Tartu (Estonia), the Lviv Polytechnic National University, University of Turin (Italy) and Pierre and Marie Curie University – Paris 6 (France).

NANO-2023 was the 11th conference in the series of NANO-conferences initiated by the Institute of Physics of NAS of Ukraine in 2012 in the framework of FP7 Nanotwinning 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 2014-2017, 450 scientists took part and in 2018 it gathered above 650 participants. In 2021 conference was attended by more than 700 scientists 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 2021 and 2022 the Organizer Committee has received more than 500 application forms from about 25 countries of the world each years.

The NANO-2023 conference brought together leading scientists and young researchers from many countries of the world. This year its topics were as follows: Nanobiotechnology for health-care; Nanochemistry and biotechnology; Nanocomposites and nanomaterials; Nanoobjects microscopy; Nanooptics and photonics; Nanoplasmonics and surface enhanced spectroscopy; Nanoscale physics; Nanostructured surfaces; Physico-chemical nanomaterials science.

Website of the NANO-2023 conference: <http://nano-conference.iop.kiev.ua>

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## **Welcome to International Conference «NANOTECHNOLOGY AND NANOMATERIALS»!**

It gives me a great pleasure to welcome you all at the International Conference “Nanotechnology and nanomaterials” (NANO-2023) that will be held in Lviv from August 16 to 19, 2023. Its aim is to promote scientific contacts and discussions between researchers representing various fields.

Previous NANO Conferences, held in Ukraine in 2013-2022, allowed the participants, including young scientists, to familiarize with current research and application problems in this area and thus forward implementation of nanotechnologies into innovations meeting public needs. The events also gave the opportunity to young and early-career researchers to attend lectures of internationally recognized experts and roundtable discussions on the emerging fields in nanosciences and nanotechnologies.

Our previous International Conferences and Summer Schools received positive feedback from international experts and from the media. Now we are holding the 11<sup>th</sup> such meeting, for which we are deeply grateful to its indefatigable initiator and organizer, Dr. Olena Fesenko and all her assistants, as well as to the universities and institutes that hospitably welcome the participants.

This year above 600 registration forms have been received from scientists representing more than 30 countries. We especially appreciate the participation in the conference of our foreign colleagues, both those who attend here and those who communicate their works remotely.

The fruitful cooperation of scientists is highly important not only to science itself. It helps us to overcome political and war conflicts and misunderstandings and to find our just peaceful future, which is now vitally important not only to Ukraine but also to other countries.

I wish the participants of the Conference to successfully share and broaden their knowledge in nanoscience and nanotechnologies, to advance the networking and launch new contacts between academia and research players in this area and thus to create a good basis for further practical contributions.

May good health serve us and promote creative success in our research!

Academician of NAS of Ukraine,  
Professor



**Anton G. Naumovets**

## Electronic and optical properties of of $\text{AgXBr}_3$ ( $\text{X} = \text{Ca}$ and $\text{Sr}$ ) Perovskites: An ab initio study with the Tran–Blaha-modified Becke–Johnson density functional

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In this study, we conducted an ab initio investigation of the structural, electronic and optical properties of  $\text{AgCaBr}_3$  and  $\text{AgSrBr}_3$  Calcium-based halide perovskites. using the full-potential linearized augmented plane-wave (FP-LAPW+lo) method [1] basis set as implemented in the WIEN2k code [2]. Calculated structural parameters, including the lattice constants ( $a$ ), bulk modulus ( $B$ ) and its pressure derivative ( $B'$ ), for the considered compounds using both the local density (LDA) [3] and generalized gradient approximations (GGA–PBEsol) [4] are consistent with the available data in the scientific literature. To calculate the electronic properties, the exchange-correlation potential is treated with various functionals, and we find that the newly developed Tran–Blaha-modified Becke–Johnson (TB-mBJ) [5–7] functional significantly improves the band gap. Band structure, total and site-

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