



2nd INTERNATIONAL SYMPOSIUM

"NONCOVALENT INTERACTIONS IN SYNTHESIS, CATALYSIS, AND CRYSTAL ENGINEERING"

(NCI-2022)

Moscow, 14-16 November 2022

BOOK OF ABSTRACTS

ISBN 978-5-6045474-9-6



9 785604 547496

In the framework of the Russian Academy of Sciences initiative
“Towards the 300th anniversary of the Russian Academy of Sciences”

ORGANIZERS

A.N. Nesmeyanov Institute of Organoelement Compounds RAS

Institute of Chemistry, Saint Petersburg State University

Tomsk Polytechnic University

N.S. Kurnakov Institute of General and Inorganic Chemistry RAS

N.D. Zelinskii Institute of Organic Chemistry RAS

COMMITTEES

Co-Chairs

Kukushkin V.Yu.

Shubina E.S.

Resnati G.

Ananikov V.P.

Vatsadze S.Z.

Gorbunova Yu.G.

Trusova M.E.

Filippov O.A.

Yusubov M.S.

Academic secretaries

Postnikov P.S.

Filippov O.A.

Zlotin S.G.

Karasik A.A.

Martynov A.G.

Postnikov P.S.

Program Committee

Shubina E.S. – chair

Vatsadze S.Z.

Martynov A.G.

Organising Committee

Belkova N.V. –

Deputy chair

Alabugin I.

Prikhodchenko P.V.

Tkatchenko A.

Tolstoy P.M.

Trifonov A.A.

Tolstoy P.M.

Postnikov P.S.

Filippov O.A.

TECHNICAL SUPPORT



PROFESSIONAL
CONGRESS ORGANISER
WWW.MESOL.RU

Theoretical insights on non-covalent interactions in functional materials

Olga A. Syzgantseva

*Lomonosov Moscow State University, 119992, Moscow, Leninskie Gory 1-3, Russia
e-mail: osyzgantseva@gmail.com*

Non-covalent interactions (NCI) are playing a major role in the creation of functional materials in various fields ranging from hybrid organic-inorganic systems to polymer composites. In particular, halogen and pnictogen bonds are crucial for the crystallization and self-assembly of various materials. In this talk, the role of non-covalent interactions in the formation of the hybrid 2D lead halide perovskites and their interfaces with 3D counterparts is analyzed using theoretical modeling. The topological descriptors of the electron density are employed for the visualization and quantification of the NCI in these compounds. The relationships between the NCI descriptors, the crystal structure and the interaction energies within these compounds are investigated. This analysis provides useful insights on the mechanisms and trends in the formation of the hybrid 2D perovskites and their interfaces, needed for the design of novel perovskite-based materials for optoelectronics and photovoltaics.

Acknowledgements

The research is carried out using the equipment of the shared research facilities of HPC computing resources at Lomonosov Moscow State University. The Siberian Branch of the Russian Academy of Sciences (SB RAS) Siberian Supercomputer Center is gratefully acknowledged for providing supercomputer facilities.