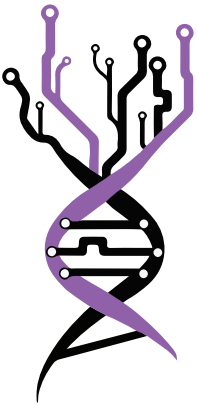
#BelBi2023 • Belgrade, Serbia

BOOK OF ABSTRACTS



4th Belgrade Bioinformatics Conference

HYBRID • 19 - 23 JUNE **2023**

EDITORS
Dr. Ivana Morić
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ISBN: 978-86-82679-14-1

belbi.bg.ac.rs

Title 4th Belgrade Bioinformatics Conference
BOOK OF ABSTRACTS

Publisher Institute of Molecular Genetics and Genetic Engineering, University of Belgrade
Vojvode Stepe 444a, Belgrade, Serbia
https://www.imgge.bg.ac.rs/

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Technical editor Dušan Radojević

ISBN **978-86-82679-14-1**

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FOREWORD

Dear colleagues and friends,

The 4th Belgrade Bioinformatics Conference - BelBi2023, where many high-quality scientific contributions were presented, has just ended. With great thanks to all participants, we now proudly present a book of abstracts that both reflects the scientific abundance and diversity of the conference and serves as a reminder of a memorable event.

Several research institutions, faculties, and scientific societies from Serbia joined forces in organizing this international conference, which covered numerous topics in computational biology, bioinformatics, and biomedical and health informatics. The main goal of BelBi2023 was to foster contact between scientists, both early stage career and senior researchers, allowing them to share experiences and latest advances in their fields. We sincerely hope that BelBi2023 has served as a platform for researchers from around the world to meet, initiate new collaborations, and expand professional contacts, and that all of you would become a part of the growing BelBi community.

We are grateful and proud to have welcomed more than 250 researchers from 21 countries. We have had 28 scientific sessions, consisting of more than 60 lectures (including eight Keynote talks), 47 presented posters, as well as three workshops and one satellite event – COST action. We have also organized seven industry lectures, including the NGS Challenge, two Meet the Expert Sessions, and one Business Coffee Break where ten start-up companies took part. And finally, the future BIO4 campus was presented and first panel on Serbia's resources for storage and analyses of genetic data was organized.

We would like to thank all the members of the International Advisory Board and the International Program Committee for their efforts and help in making this event a success. We are very grateful to the Ministry of Science, Technological Development and Innovation of the Republic of Serbia, SAIGE project, and UNDP-Serbia for their support. Finally, the Local Organizing Committee is very grateful to all the sponsors of the conference - BGI, Illumina & Elta'90MS, PacBio & East Diagnostics, ThermoFisher Scientific & Vivogen, Huawei, Labena, DSP Chromatography, RNIDS, Telekom Srbija, Alfa Genetics, Kefo and Superlab, hoping that they will stay with us for many years to come.

Looking forward to seeing you again at the 5th Belgrade Bioinformatics Conference.

Belgrade, July 2023

Dr. Valentina Đorđević
& Dr. Ivana Morić,
On behalf of BelBi2023
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Energy and information exchange between "donor" and "molecular bridge" structures: non adiabatic polaron model

Dalibor Chevizovich[1], Vasilije Matic[1]*, and Zeljko Przulj[1]

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Molecular chains (such as protein chains with alpha-helical secondary structure, DNA and RNA molecules) can play the role of "bridges" for the highly efficient transfer of various types of submolecular excitations (vibron excitations or electrons) over very long distances (comparable to the length of the molecular chain itself). In the case when this process takes place in living cells, the biomolecule is placed in an environment where it is usually in thermodynamic equilibrium with the "heat bath". As a result, the structural elements of the molecular chain perform mechanical oscillations. In the general case, such mechanical oscillations disrupt the ability of the molecular bridge to transfer the excitation over a longer distance.

On the other side, by interacting with the thermal oscillations of the structure, excitations injected into the molecule may be trapped and can form a stable self-trapped (polaron-like) state. Such quasiparticles can move through the structure with minimal energy loss. In this way, the high efficiency of energy and charge transport in living cells can be explained. However, the properties of the possibly formed polaron quasiparticle must also be affected by the presence of the donor molecule.

Here, we have discussed the mechanism of excitation transfer from a molecular structure (donor molecule) to the molecular chain. The presence of the donor structure and the temperature influence on the energy of the self-trapped excitation were considered in the dependence of the basic energy parameters of the molecular bridge. The obtained results indicate the possibility of the formation of two types of self-trapped states: a quasi-free excitation, which can easily move through the molecular bridge, and a localized, practically immobile excitation, which is similar to a non-adiabatic polaron quasiparticle.

Keywords: energy transfer, information transfer, biomolecular structures, self-trapping, polaron quasiparticle

Acknowledgment: Supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia and by the Project within the Cooperation Agreement between the JINR, Dubna, Russian Federation and Ministry of Education and Science of the Republic of Serbia.

ISBN: 978-86-82679-14-1