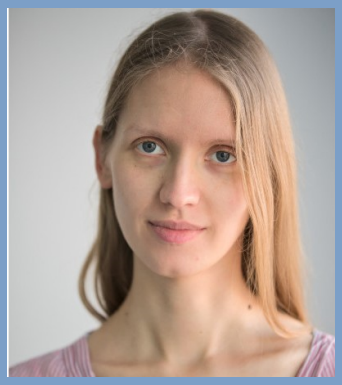


ÉVA ZSUZSANNA MIHÁLKA

Faculty of Natural Sciences
Comenius University

Project number
3154/01/02

Project duration
10/2021 - 9/2025
Interruption
5/2022 - 5/2023

BIOGRAPHY

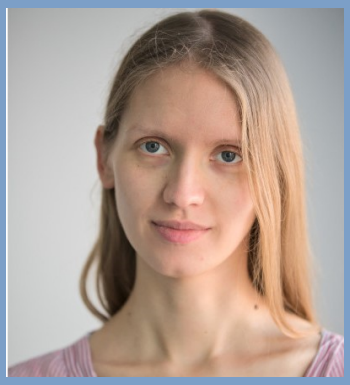
I studied mathemathics and chemistry at Eötvös Loránd University (ELTE), Budapest, Hungary. Following the masters degrees, I obtained my PhD degree in 2021, working in the Laboratory of Theoretical Chemistry at ELTE, under the supervision of Péter. R. Surján and Ágnes Szabados.

"The SASPRO 2 fellowship was an opportunity with perfect timing, as it offered an excellent postdoctoral career path rigtht after my PhD studies. The position at Comenius University is my first postodctoral fellowship, and my main reasons for applying were the possibility of learning from and working with my prospective SASPRO 2 supervisor, Prof. Jozef Noga, as well as the prestigious nature of the fellowship, opening new doors in my scientific career. It presented an opportunity to put the knowledge I obtained during my PhD years in a different perspective and utlize my skills in a new context, while simultaneously evolving in my respective research area.
Accordingly, I expect that during this period I can develop as an individual researcher, get more immersed in the international community of my field, obtain new science-related skills, and expand my scientific network thanks to the stable background offered by the fellowship and the host organisation. With the support from the SASPRO 2 programme, I can carry out my research in a very inspiring scientific environment, which in turn will help me become a more accomplished scientist and advance my future career prospects as well.

PROJECT SUMMARY

Geminal-based references in explicitly correlated frameworks

Knowing the electronic structure of atoms and molecules helps to better understand or even predict chemical and physical phenomena around us. Balancing qualitative and quantitative accuracy as well as computational effort is a delicate problem, proving to be a challenge to this day. The research project aims at developing a framework which unifies two methodologies to obtain a new approach to the electron correlation problem.
The model combines explicitly correlated (denoted as F12) methods with a pair function based reference. By incorporating the interelectronic coordinate explicitly in the wavefunction Ansatz, F12 methodologies are known to increase accuracy of numerical results and significantly reduce the corresponding computational cost, as a consequence of a qualitatively improved wavefunction. F12 frameworks are able to recover dynamic part of electron correlation.
On the other hand, models based on pair functions (geminals) offer an efficient but powerful tool to describe the static contribution to the correlation energy. The reference, obtained as an antisymmetrized product of geminals, describes intra-pair correlation in an exact manner. Preliminary results point to the feasibility of employing geminal-based references within an explicitly correlated framework, both in terms of numerical accuracy and algorithmic complexity.
The proposed project is intended to explore the advantages of this unified approach, by combining the experience of the supervisor in explicitly correlated methods and the knowledge of the applicant in geminal-based theories.



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PUBLICATIONS

1. J. Chem. Theory Comput. 17, 4122 (2021) https://pubs.acs.org/doi/10.1021/acs.jctc.1c00305
2. J. Chem. Theory Comput. 16, 892 (2020) https://pubs.acs.org/doi/10.1021/acs.jctc.9b00858
3. J. Chem. Phys. 150, 031101 (2019) https://aip.scitation.org/doi/10.1063/1.5083191

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