Anton Pershin

Curriculum Vitae

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1034 Budapest, Hungary
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Date of birth: 18.02.1987
Married, 1 child
Citizenships: Hungary, Russia

Education

2010–2013 **Ph. D. in Theoretical Chemistry**, Institute of Physical and Theoretical Chemistry, University of Regensburg (UR), Germany.

2008–2009 **M. Sc. in Physical Chemistry**, Department of Chemistry, V. N. Karazin Kharkiv National University, Ukraine, *diploma with honours*.

2004–2008 **B. Sc. in Physical Chemistry**, Department of Chemistry, V. N. Karazin Kharkiv National University, Ukraine, *diploma with honours*.

PhD thesis

title Development and application of multiscale modeling techniques for studying the loss processes in polymer-based solar cell nanodevices
supervisor Stephan A. Baeurle

Employment history

2019-present **Research Fellow**, Wigner Research Centre for Physics, Budapest, Hungary
Theory of quantum bits in diamond and 2D materials, supervisor *Adam Gali*

2017–2019 **Marie Curie Researcher**, Laboratory for Chemistry of Novel Materials, University of Mons, Belgium.
Theoretical rationalization of TADF process in solid state, with *Yoann Olivier* and *David Beljonne*

2016–2017 **FRNS Postdoctoral Fellow**, Laboratory for Chemistry of Novel Materials, University of Mons, Belgium.

Modeling of photo-switchable molecules on 2D materials, supervisor *David Beljonne*

2013–2015 **Postdoctoral Fellow**, Laboratory of Theoretical Chemistry, Institute of Chemistry, Eotvos Lorand University (ELTE), Budapest, Hungary.

Excited state behavior and charge transport properties of pi-conjugated organic systems, supervisor *Peter G. Szalay*

2010–2013 **Research Fellow**, Institute of Physical and Theoretical Chemistry, University of Regensburg, Germany.

Development of multiscale approaches for the polymer solar cells, supervisors *Stephan A. Baeurle and Bernhard Dick*

2009–2010 **Research Fellow**, Institute of Combinatorial Organic Chemistry of Biologically Active Substances, Kharkiv, Ukraine.

Synthesis of biologically-active compounds, supervisor *Sergey N. Kovalenko*

Awards and external funding received

2020 2DQubits project (with Adam Gali) was given 3M core-hours of CPU via PRACE call.

2017 Individual Marie Curie Fellowship (178.000 euro)

2016 Belgian FRS-FRNS postdoctoral fellowship (138.000 euro)

2015 MTA postdoctoral fellow from Hungarian Academy of Science (28.000 euro)

2015 Short-term scholarship from Action Austria-Hungary (300 euro)

2015 Travel grant from Dynasty Foundation (500 euro)

2014 Travel grant from Action Austria-Hungary (300 euro)

2009 3rd place at "Chemical Karazin Readings 2009"

2007 Award "For academic excellence and active participation in social, scientific and creative activities of V. N. Karazin Kharkiv National University"

Teaching experience

2015 "Monte Carlo methods in Chemistry" for PhD students, ELTE

2015 "Advanced Physical Chemistry: Quantum Chemistry" (with P. Szalay), ELTE

2014 "Methods of Quantum Chemistry" (with P. Szalay), ELTE

2011–2013 Practical training in Physical Chemistry for undergraduate students, UR

Supervision/coaching of students

BSc: MJA Christlmaier; **PhD**: R Dilmurat, D Hall, G Londi, S Donets; **Postdoc**: A Slassi, SM Gali

Presentations at scientific conferences

2022 Defects in solids for quantum technologies, Sweden

2022 APS March Meeting, USA

2018 International School on 2D Materials, Cargese, France

2015 Central European Symposium on Theoretical Chemistry, Banska Bystrica, Slovakia

2015 15th Fock Meeting, Vladivostok, Russia

2014 Central European Symposium on Theoretical Chemistry, Nagyborzsony, Hungary

2014 50th Symposium on Theoretical Chemistry. Vienna, Austria

2013 DPG-Frühjahrstagung, Regensburg, Germany

2012 48th Symposium on Theoretical Chemistry, Karlsruhe, Germany

2012 Bunsentagung, Leipzig, Germany

2012 DPG-Frühjahrstagung, Berlin, Germany

2009 Chemical Karazin Readings, Kharkiv, Ukraine

2008 Chemical Karazin Readings, Kharkiv, Ukraine

2007 X International Conference on the Problems of Solvation and Complex Formation in Solutions, Suzdal, Russia

2007 Chugaev XXIII International Conference on the Coordination Chemistry, Odessa, Ukraine

Participation in research projects

2019-2022 H2020, project ASTERIQS

2016-2018 M.ERA-Net, project MODIGLIANI

2013-2015 Hungarian Scientific Research Fund (OTKA) (No. 104672)

2010-2013 Deutsche Forschungsgemeinschaft (DFG) (No. BA 2256/3-1)

Recent collaborations

Jean-Christophe Charlier, UC Leuven, Belgium

Eli Zysman-Colman, University of St Andrews, Scotland

Paulo Samori, University of Strasbourg, France

Richard Friend, University of Cambridge, England

Akshay Rao, University of Cambridge, England

Luca Muccioli, University of Bologna, Italy

Juan-Carlos Sancho-Garcia, University of Alicante, Spain

Hiroyuki Tamura, University of Tokyo, Japan

Language skills

English (fluent), *German* (fluent), *Hungarian* (intermediate), *Russian* (mother tongue), *French* (beginner), *Ukrainian* (advanced)

Referees

Prof. Dr. David Beljonne, Department of Chemistry, U Mons. david.beljonne@umons.ac.be

Prof. Dr. Yoann Olivier, Department of Physics, U Namur. yoann.olivier@unamur.be

Prof. Dr. Peter G. Szalay, Department of Chemistry, ELTE. szalay@chem.elte.hu

Editorial

2020-2022 Editorial Board member of Advanced Materials Science and Technology

Research skills

By the time of application, I have demonstrated an excellent commitment to conducting independent and groundbreaking research. Of my ~37 publications, 15 are with a "special" authorship (first, last or corresponding author). 13 papers are published in top journals with a high impact factor (IF> 10) including leading journals for materials science and solid state physics, such as Nature (2 publications), Nature Materials, Nature Communications, Advanced Materials, npj Quantum Information, and others [3 of them are as the first author]. After a successful PhD defense in Germany, I conducted postdoctoral research with world-class scientists, namely PG Szalay (h-index 56 from Google Scholar), D Beljonne (h-index 107) and A Gali (h-index 66) in two different

countries. Whenever possible, I actively participated in the teaching activities of the host universities, both by preparing lectures and seminars for ongoing courses, and by planning my own course for ELTE graduate students (concerning the use of Monte Carlo methods). Working on various domestic and international projects, I have developed an interdisciplinary vision in many areas, which includes computational materials science, solid state physics, and quantum information theory. As a researcher, I successfully completed an Individual Marie Curie project and developed good resource management skills when I successfully applied for major (international) research and travel grants in my current academic position. Moreover, I have already demonstrated leadership and team management skills and the ability to motivate early-stage researchers. This is proven by the fact that we published joint publications with all my seven supervised students.

My research profile is characterized by a strong multidisciplinary character and a broad range of research interests in materials science. In my career of theoretical materials scientist, I acquired the mastery of various modelling techniques (from physical chemistry, solid state physics, and soft matter), which have been successfully employed to explain experimental data or even predict novel phenomena. I distinguish myself for key achievements in the fields of low-dimensional and molecular functional materials, and for a highly propositive participation in various international collaborations. My research bridges the rigorous approaches of physical sciences, with the ambition to quantitatively describe systems of high complexity from a chemical and structural point of view. On the technical side, I possess the expertise and unique know-how in modeling the defect qubits by the highly correlated electronic structure methods (for instance, the coupled cluster theory, CC), in the characterization of interfaces between the molecules/defect qubits and the environment, and in modeling of the spin-conversion processes.

5 selected publications from the last five years

[1] **Highly emissive excitons with reduced exchange energy in thermally activated delayed fluorescent molecules**

Anton Pershin, D Hall, V Lemaur, JC Sancho-Garcia, L Muccioli, E Zysman-Colman, D Beljonne, and Y Olivier

Nature Communications, 2019, 10, 597

Short description: with a new design strategy, we demonstrate that the TADF emitters can have a bright and narrow PL signal. This paper is groundbreaking in the field of TADF OLEDs as it allowed for a step-change in the external quantum efficiency.

My contribution: main idea, all calculations, drafting the paper.

[2] Dielectric control of reverse intersystem crossing in thermally-activated delayed fluorescence emitters

A Gillet*, **Anton Pershin***, R Pandya, S Feldmann, AJ Sneyd, E Evans, T Thomas, L Cui, A Alvertis, B Drummond, GD Scholes, Y Olivier, A. Rao, R. Friend, and D Beljonne

Nature Materials, 2022, 21 ***contributed equally**

Short description: a joint experimental-theory paper for the excited state dynamics in organic emitters. With an original multiscale modelling aprroach for the excited states, we show that the environment can selectively change the intersystem crossing rates between states by orders of magnitude (nowadays, used to fine-tune the alignment of the excited states).

My contribution: all calculations, drafting the paper.

[3] Highly tunable magneto-optical response from MgV color centers in diamond

Anton Pershin, G Barcza, O Legeza, and A Gali

npj Quantum Information, 2021, 7, 99

Short description: we identify an origin of a new photostable PL signal in diamond as related to a MgV^{-}, defect. We show how to use it as a qubit for the quantum information technology.

My contribution: DFT and CASSCF calculations, drafting the paper.

[4] Interlayer Bonding in Two-Dimensional Materials: The Special Case of SnP_3 and GeP_3

A Slassi, SM Gali, **Anton Pershin***, A Gali, J Cornil, and D Beljonne*

The Journal of Physical Chemistry Letters, 2020, 11, 11, 4503–4510 **[*corresponding author]**

Short description: we show that structural defects can induce chemical bonding between the layers of 2D materials. This leads to an enormous modification of optical and transport properties.

My contribution: main idea; supervision of A. Slassi and S.M. Gali; DFT, GW/ Bethe–Salpeter equation (BSE), and transport calculations; drafting the paper.

[5] **The role of charge recombination to spin-triplet excitons in non-fullerene acceptor organic solar cells**

A Gillett, A Privitera, R Dilmurat, A Karki, D Qian, **Anton Pershin**, G Londi, W Myers , J Lee , J Yuan, SJ Ko, M Riede, F Gao, G Bazan, A Rao, TQ Nguyen, D Beljonne, and R Friend

Nature, 2021, 597, 666–671

Short description: We show that the hybridization between donor and acceptor units can suppress the efficiency losses caused by a non-geminal recombination process. This idea comes from theory and is further supported by the experimental results.

My contribution: I conceived the theory part, supervised R Dilmurat, performed the DFT calculations for the matrix elements and rate constants, drafted the theory part.

Citations & related metrics

Total number of papers:	**37** (plus 1 preprints)
Number of papers as first/last/corresponding author:	15 (11/2/2)
Number of papers in the last 5 years:	26 (plus 1 preprints)

Total # of citations: 942 (Scopus), 937 (WoS), 936 (MTMT), 1190 (Scholar)

h-index: 13 (Scopus), 13 (WoS), 14 (MTMT), 15 (Scholar)

Independent citations (MTMT): 767

Effective independent citations (MTMT): **527.5**

Cumulative impact factor: **~396**

Google scholar profile: https://scholar.google.be/citations?user=Rqtf1AwAAAAJ&hl=en

Research plan for the next three years

Quantum computing has the potential to radically transform a wide variety of industries. While the technology has reached the proof-of-concept stage, scalability challenges loom ahead. To achieve the full potential of quantum computing, a way of building large-scale and reliable quantum computers is still to be found. To this end, electronic spins in solid state systems are one of the most promising technological foundations for building a quantum computer. So far, a few qualified materials, such as spins in silicon carbide and nitrogen-vacancy centers in diamond, were suggested. Building on decades of research and development in material sciences and quantum optics, quantum systems with a limited number of qubits can be efficiently controlled nowadays. However, despite this great success, construction of large quantum networks (essential to achieve the quantum supremacy) is still hampered by the inflexibility of the underlying host materials.

Moreover, a successful qubit for quantum computing should fulfill a number of requirements, such as stable zero-phonon line; large zero-field splitting parameters; spin-selective transitions; large Debye-Waller factors; possibility of optical readout for the spin-states. The typical point defects in solids exhibit only a fraction of the favorable features, while the remaining properties are hard to alter. By contrast, my aim is to develop a framework for an all-organic qubit system that can be controlled with light, yielding precisely engineered single-site properties. An appealing facet of this molecular-based approach is the opportunity to independently tune these intrinsic properties by modifying the matrix molecules and thus selectively enhance individual characteristics. A few examples of organometallic compounds illustrated the feasibility of optically addressable molecular qubit materials. The use of all-organic qubits can prevent the development of large spin-orbit interaction, which in turn limits the spin-coherence time.

Given a large chemical space of possible candidates, theoretical calculations are needed to identify the possible qubits. However, in the literature, there is no consensus about the electronic structure method, which can be used to reliably predict the properties of correlated states of the qubits. The aim of my research is therefore twofold. First, an efficient electronic structure method is to be found among the post-Hartree-Fock approaches and is to be directly extended to the crystalline environment to model the qubits using the plane waves. Here, by applying the existing solutions for molecules, calculations of the key qubit properties in solids will also be implemented.

Noteworthy, I have already developed an approach to perform the high accuracy correlated calculations in the plane wave basis with an arbitrary post-Hartree-Fock method, which has been tested for many systems with great success [the paper is close to be submitted]. Second, the identified method will be applied to search for the qualified candidates among the stable organic biradicals. The computed structure-property relationship will be then used to deliver the design rules for the chemical structures of qubits and host matrices. I plan to execute this research as a part of an ongoing collaboration with the NVision Imaging Technologies GmbH (Germany) who will implement the most promising structures, also ensuring the experimental feasibility of the proposed systems.

Year 1: *Benchmark calculations for the excited states*. First, a suitable multireference method, used to accurately describe the correlated qubit wavefunctions in the organic crystals, will be chosen. The reference wavefunctions will be computed using the projector augmented wave method, implemented in VASP. The molecular integrals will be then exported in the FCIDUMP format and directly used by the ab initio codes (PySCF, MRCC, Budapest-DMRG, etc). My preliminary results show a high efficiency of this approach, e.g. systems of ~100 carbon atoms are trackable at the coupled cluster singles and doubles (EOM-CCSD) level of theory. A pool of electronic structure methods will consist of n-electron valence state perturbation theory (NEVPT2), restricted active space density matrix renormalization group (RAS-DMRG), multiconfiguration pair-density functional theory (MC-PDFT), etc. To test the methods, the benchmark calculations will be performed for several excited singlet and triplet states using the reference molecular databases (e.g. Thiel's set, QUEST, etc). For the selected method, the excitation energies, calculated using large clusters and fully periodic models of the potential organic qubits (stable carbenes) in solid state, will be compared to the available experimental data.

Year 2: *Improved interface to the excited state codes and first-order properties.* Beside the excitation energies, the molecular integrals enable to compute the reduced density matrices which will be used to calculate the state properties. The transition moments will be calculated as the expectation values from the transition densities, so also the spin-spin couplings and spin-orbit coupling matrix elements. Note that the respective integrals between the crystal orbitals are accessible from VASP using the standard processing tools. Similarly, the calculation of forces in the ground- and excited-state will be achieved using the Hellmann–Feynman theorem. The calculated properties will be verified for the molecular databases. A direct interface for the on-the-

fly generation of the molecular integrals will be also developed to enable an efficient treatment of large systems. As a result, a toolkit for calculating the key properties of the organic qubits, such as various decay rates including the relaxation effects, will be developed.

Year 3: *Structure-property relationship for the organic qubits.* The qubit materials will be taken from the Cambridge Structural Database to identify a pool of qualified molecular matrices that will be subjected to computational screening. The prototype scaffolds for this search are mono- and biarylketones. The parameter space to tune the *D*/*E* zero-field splitting parameters, electronic absorption/emission profiles, as well as magnetic coupling includes $R_2C=O$ headspace, radius dependent hydrogen densities, C-C-C and torsional angles; number of independent molecules and unique orientations per unit cell, as well as hydrogen- and packing density and intermolecular distances. The resulting pool of candidates will be subjected to the selected high-level ab initio method to evaluate the key parameters for the qubits, including *D*/*E* constants, fluorescence- and intersystem crossing rates. For the selected systems, unfavorable characteristics of the qubit, such as spectral diffusion, inhomogeneities, insufficient inhomogeneous broadening, inapt absorption and emission profiles, will be analyzed to develop the most efficient molecular design strategies. This effort will enable identification of the structural features that are responsible for the unwanted behavior and will ultimately guide the synthesis of the modified qubits and host matrices by the experimental partners.

Funding acquisition plans

In the future, I plan to setup an independent group at Wigner RCP though applying for the external funding sources. I have already tried with the ERC starting grant, which was well received by the panel members (mark "B" in the first round), yet not funded. My plan is to re-apply for an ERC grant in the upcoming years, considering the comments of the panel. The "Momentum" program is regarded as an alternative option, which I am planning to explore. Different processes have been launched to build up to a successful research profile within the Hungarian system. Thus, I have an ongoing application for the Bolyai fellowship. Recently, I was accepted as a PhD supervisor at György Hevesy Doctoral School (ELTE). I will also apply for a of title of Doctor of the Hungarian Academy of Sciences in the next years.