Curriculum Vitae

Name:	Pietro Faccioli
Date and Place of Birth:	February 14-th 1974, Verona, Italy.
Citizenship:	Italian.
Current Position:	Associate Professor
Working Address:	Dipartimento di Fisica "G. Occhialini", U. Milano Bicocca Piazza della Scienza 3, 20126, Milano (Italy)
Phone:	+39 -340-308-7658
Email:	`pietro.faccioli@unimib.it`
URL:	https://sites.google.com/unimib.it/pietro-faccioli
Other Affiliations :	Italian Institute for Nuclear Physics (INFN)

Education, Training, and Occupations

Academic Degrees

- Undergraduate Degree in Physics earned "*summa cum laude*" at the Trento University (1998).
- Ph.D in Physics, SUNY at Stony Brook, USA (2002).

Extended Periods in Foreign Institutions

- 2003, 2005, 2006, 2007, 2009: "Bruno-Rossi" visiting scientist in the Center for Theoretical Physics of the Massachusetts Institute for Technology (USA)
- 2009: Visiting scientist at IPhT CEA-Saclay (France): 10 months.
- 1999-2002: Ph.D student at SUNY Stony Brook (USA): 3 years
- 1996: Exchange student at Imperial College (London): 10 months

Present and Past Occupations

- Since 2023: Associate Professor at the Physics Department of University of Milan-Bicocca.
- 2014-2023: Associate Professor at the Physics Department of Trento University.
- 2006-2014: Tenure Junior Faculty at Trento University (Ricercatore Confermato).
- 2005-2006: Tenure Track Junior Faculty at Trento University.
- 2002-2005: Postdoctoral Associate at European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT*).
- 1998-1999: Junior Research Fellow at European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT*).

Italian Habilitations (ASN) for Full Professor Position

- 02/A2 (GSD code: 02-Phys-02): Theoretical physics of fundamental Interactions
- 02/B2 (GSD code: 02-Phys-04): Theoretical physics of condensed matter
- 02/D1 (GSD code: 02-Phys-06): Physics applications to biology, medicine, and cultural heritage.

Institutional Roles and Responsibilities

- International scientific spokesperson for the Zeprion-1 and Zeprion-2 experiments (2021-2025). International PI of the "ZePrion-2" project proposal, approved by the European Space Agency, within the BSGN program (2024).

- National PI of the PRIN grant "Functional Role of Protein Folding Intermediates: A Cross-Disciplinary Study Integrating Molecular Simulations with Biophysical and Biochemical Experiments" (2023).

- Founder of a research group devoted to application of computational physics methods to molecular biology at U. Trento, leading to hiring 3 tenure professors (2007-2023).

- Coordinator for the Trento group of the "BIOPHYS" scientific initiative of INFN for research in computational biophysics (2014-2023).

- Coordinator for the Trento group of the "AD31" (2008-2013) and "NINPHA" scientific initiative of INFN for research in hadron physics (2015-2016).

- Involved in the setting of the M.S. Degree in Quantitative and Computational Biology, Trento University (2015-2016).

- Member of the co-ordination board of the M.S. Degree in Quantitative and Computational Biology, Trento University (2016- 2023).

- Member of the co-ordination board (Collegio Docenti) of the Doctoral School in Physics, Trento University (2015-2023).

- Member of the Collegio Docenti of the Doctoral School in Physics and Astronomy, Milan-Bicocca University (since 2023).

- Member of the Collegio Docenti of the Industrial Doctoral School in Strategic Innovation for Sustainable and Smart Ecosystems Milan-Bicocca University (since 2023).

Non-Academic Roles

- Scientific coordinator and spokesperson of the ZePrion international collaboration (2021-2025).

- Co-founder of Sibylla Biotech SRL (www.sibyllabiotech.it), inventor of the underlying computational technology for molecular simulations, co-inventor of the underlying drug discovery approach (see "Patents") and scientific advisor (since 2017).

Awards and Recognitions

- Sibylla Biotech SRL was selected among the 8 world finalists of the Nature Merck Spinoff Prize[1] (2021).
- Invited delegate of the Italian Ministery of Foreign Affairs to represent "Italian excellence in scientific and technological innovation" at the *'Ita-Usa Innovation Forum"* (Stanford U.) on the occasion of the formal visit of the President of the Italian Republic, On. Sergio Mattarella (2019).
- "V. Gribov Prize for Young Talents in Theoretical Physics", Erice (Italy) (2001).

Grants

- "Zeprion-II" BSGN-ESA Advanced Acceleration Grant: 100 kEur (2024): International PI/spokesperson
- PRIN Grant: 270 kEur (2023): main proponent/national PI
- Quantum@TN Grant covering one Ph.D fellowship (2021): co-PI
- "Ramon Foundation Grant" covering the allocation of the astronaut's time and the transportation cost to the International Space Station of the experimental equipment of the ZePrion Experiment. Estimated cost 250 kEur (2020, declined): Pi
- Research agreement between INFN and Sibylla Biotech, leading to 1 million CPU hours on CINECA supercomputing facilities to perform folding simulations for ACE2 protein (2020): co-PI
- INFN-TT "Research for Innovation 2019" grant covering one-year post-doctoral fellowship (2019): PI
- Quantum@TN Grant covering one Ph.D fellowship (2018): co-PI
- Trento University special grant for high-priority projects ("Grandi Progetti di Ateneo") for 40 kEur (2015): co-PI
- Alpha-1 Foundation grant, sub-contracting for 20 kEur form U. Maryland at Baltimore (2014): PI
- CNRS grant supporting a long-term visit at the IPhT of CEA-Saclay (France) (2009)
- "Bruno-Rossi" grant within the INFN-MIT exchange program (2003, 2005, 2006, 2007, 2009).

[1] "Turning transient structures into drug targets", Nature Outlook 24 June 2021. "Disrupting protein folding to tackle cancer", Nature Outlook 24 June 2021.

Scientific Productivity and Metrics

- 86+ peer-reviewed publications, more than 70% of which as first or corresponding author (in more than 50% of the remaining papers, the authors are listed is in alphabetic order). Fraction of peer-reviewed publications coauthored by the PhD advisor $< 10\%$. Fraction of peer-reviewed publications coauthored by the MS thesis advisor: $< 10\%$.
- Number of filed patents: 2. Number of granted patents: 2.
- Broadness and cross-disciplinarity. Papers published on:
  - Generalist journals: P.N.A.S., Science Advances, and Scientifc Reports
  - Specialized journals on *physics*: Phys. Rev. Lett., Phys. Rev. A, B, C, D, E, and X Life. Nucl. Phys. A and C, Phys. Lett. B, Biophys. J., J. Chem. Phys.
  - Specialized journals on *chemistry*: J.A.C.S., J.C.T.C., J. Phys. Chem. B, J. Biol. Chem., Macromolecules
  - Specialized journals of *life science and drug discovery*: PLoS Comp. Biol., Curr. Opin. Pharm., J. Biol. Chem., Structure, Biomolecules, PLoS Pathogens, J. Mol. Biol., Comm. Biol., Proteins, Nucleic Acid Res., and EMBO J.
- H-index = 24 (Scopus), 28 (Google Scholar). 15-year H-index (since 2010): 18 (Scopus). Total number of citations: $\geq$1906 (Scopus), $\geq$ 2833 (Google Scholar).
- Selection of 15 Publications:

1. V. Panizza, A. Roggero, P. Hauke, and P. Faccioli, Phys. Rev. Lett. 134 (15), 158101 (2025)*†
2. D. Gasparotto *et al.*, EMBO J. (2025) (DOI:10.1038/s44318-025-00567-1)†
3. F. Slongo, P. Hauke, P. Faccioli, and C. Micheletti, Science Advances 9, eadi0204 (2023)†
4. C. Micheletti, P. Hauke, and P. Faccioli, Phys. Rev. Lett. 127, 080501 (2021)†
5. P. Hauke, G. Mattiotti, and P. Faccioli, Phys. Rev. Lett. 126, 028104 (2021)†
6. L. Zanovello, M. Caraglio, T. Franosh, and P. Faccioli, Phys. Rev. Lett. 126, 018001 (2021)†
7. G. Spagnolli et al. Comms. Biol. (Nature PG) 462 (2021) †
8. M. Bondanza, L. Cupellini, P. Faccioli, and B. Mennucci. JACS 142, 21829 (2020)†
9. A. Ianeselli, S. Orioli, G. Spagnolli, P. Faccioli, L. Cupellini, S. Jurinovich, and B. Mennucci, JACS 140, 3674 (2018)†
10. S. a Beccara, L. Fant, and P. Faccioli, Phys. Rev. Lett. 114, 098103 (2015)†
11. G. Cazzolli, F. Wang, S. a Beccara, A. Gershenson, P. Faccioli, P. Wintrode, PNAS 111,15414 (2014)†
12. S. a Beccara, T. Skrbic, R. Covino, and P. Faccioli, PNAS 1092330 (2012)†
13. M. Sega, P. Faccioli, F. Pederiva, G. Garberoglio, and H. Orland, Phys. Rev. Lett. 99, 118102 (2007)

14. P. Faccioli, M. Sega, F. Pederiva, and H. Orland, Phys. Rev. Lett. 97, 108101(2006)
15. P. Faccioli and T.A. DeGrand, Phys. Rev. Lett. 91, 182001 (2003)†.

†: Corresponding or co-corresponding author. $\star$: Selected as journal's editor suggestion.

Dissemination and Outreach

- About 40 invited talks and about 60 contributed talks in international meetings.
- About 45 invited seminars, colloquia and lectures in universities and research institutions, including MIT, U. Cambridge (Dept. Applied Mathematics and Theor. Phys.), U. Cambridge (Dept. of Theoretical Chemistry *Colloquium*), U. Harvard, ETH (Chemistry *Colloquium*), National Institute for Health
- Invited lectures given at 5 international doctoral schools
- Public outreach: Divulgative lectures in science festivals (Bergamo Scienza 2023, Trieste Next 2023), featured articles in divulgative scientific journals (Le Scienze, Sapere), and featured articles or interviews in major National newspapers (Il Corriere della Sera, Il Sole 24 Ore, La Stampa, Repubblica, Panorama). Divulgative lectures in high schools (Liceo Cremona, Milan 2023).

Teaching and Mentoring

List of Courses Given

1. Machine Learning and Statistical Mechanics of Macromolecular Systems (MS in Physics, U. Milan-Bicocca)
2. Statistical Mechanics of Neural Network (M.S. in Artificial Intelligence for Science and Technology, joint course of U. Milan-Bicocca, U. Milan Statale, U. Pavia)
3. Introductory Physics (B.S. in Computer Science, U. Milan-Bicocca)
4. Macromolecular simulation in the age of machine learning (Ph.D. in Physics and Astronomy, U. Milan-Bicocca).
5. Statistical field theory (M.S. in Physics, U. Trento)
6. Quantum mechanics and quantum chemistry (M.S. in Quant. and Comp. Biol., U. Trento)
7. Macromolecular modeling (M.S. in Biotechnology, U. Trento)

8. Statistical mechanics (B.S. in Physics, U. Trento)
9. Quantum chromodynamics (Ph.D in Physics, U. Trento)
10. Introduction to nuclear and subnuclear physics (B.S. in Physics, U. Trento) – teaching assistant–
11. Classical mechanics (B.S. in Physics, U. Trento) – teaching assistant–
12. Calculus (B.S., SUNY at Stony Brook) – teaching assistant–
13. General physics (B.S. SUNY at Stony Brook) – teaching assistant–

Mentoring

- 4 post-doc supervised in theoretical physics, computational physics, and chemical physics.
- 10 Ph.D theses supervised in theoretical physics, computational physics, and chemical physics.
- 30+ M.S. theses supervised for the degrees in physics, AI for science and technology, and quantitative and computational biology.

Scholars: Several young scientists I supervised for their MS and PhD theses have had a successful academic career and earned a tenured or tenure-track positions in academic or research institutions: Roberto Covino is full professor and director of the molecular simulation sector of the Frankfurt Institute for Advanced Studies (Germany), Alan Ianeselli was tenure-track assistant professor (RTD-B) at U. Bolzano (Italy) before leaving Italy to continue his training as a research fellow at U.Yale (USA), Guglielmo Mazzola is now associate professor at SISSA (Italy), Tatjana Skrbic is now tenure researcher at U. Venezia Ca Foscari (Italy), Francesco Segatta is tenure-track professor (RTT) at U. Bologna, and Marco Cristoforetti is tenured scientist at FBK, Trento (Italy).

Participation to Selection and Evaluation Committees

- Member of the evaluation commission for tenure assignment in the Chemistry Department of ETH, Zurich (2021)
- Member of the selection committee for a non-tenure assistant professor position (RTD-A) in statistical mechanics (U. Naples Federico II) (2021)
- Member of the selection committee for a non-tenure assistant professor position (RTD-A) in high-energy experimental physics (U. Trento) (2020)
- Member of the selection committee for a tenure track assistant professor position (RTD-B) in high-energy theoretical physics (U. Trento) (2019)
- Member of the selection committee for a non-tenure assistant professor position (RTD-A) in high-energy experimental physics (U. Trento) (2020)

- External member of the Ph.D Thesis Examining Committee of the Department Physics, Florence University (2012)

- External member of the Ph.D Thesis Examining Committee of the Department of Applied Mathematics, Cambridge University, UK (2009).

Peer-Reviewing Activity

- Referee for the European Research Council (ERC) Starting Grant 2017 (proposals in computational biophysics)

- Referee for the National Science Foundation (NSF) of USA (proposals in computational biophysics)

- Referee for 20+ international journals, including Nature Communication, Physical Review Letters, Journal of the American Chemical Society, Scientific Reports, European Journal of Physics C, Physics Letters B, Physical Review D,C E, Physical Review X Life, Physical Review Research, Progress in Particle and Nuclear Physics, Journal of the American Chemical Society, Philosophical Magazine, Journal of Chemical Physics, Journal of Physical Chemistry B, New Journal of Physics, Journal of Applied Mathematics, Chaos, Journal Physical Chemistry Letters.

Organization of Conferences, Workshops, and Schools

- Co-organizer of the CECAM flagship Workshop on "Quantum computing for classical complex systems: Opportunities and challenges from soft matter to life sciences", SISSA September 2025

- Organizer of the 2nd International Workshop on "Applications of Theoretical Physics Methods in Biology", ECT* June 2010

- Co-organizer of the joint FBK-Trento University-INFN-CNR workshop on "Biophysics of Macromolecular Interactions", Trento, September 2009

- Co-organizer of the 1st International Workshop on "Applications of Theoretical Physics Methods in Biology", ECT* May 2005

- Co-organizer of the ECT* Doctoral Training Program 2006 on "Numerical Techniques in Strongly Interacting Systems", ECT* 2008.

International Collaboration Network[2]

J.-P. Blaizot (CEA-Saclay), E. Shuryak (SUNY at Stony Brook), R. Covino (Frankfurt Institute Advanced Studies), T. DeGrand (U. Colorado at Boulder), G. Ripka (CEA-Saclay), J. Negele (MIT), H. Orland (CEA-Saclay), T. Franosh (U. Innsbruck), B. Pasquali (I. Pasteur at Paris), P. Wintrode (U. Maryland at Baltimore), A. Gershenson (U. Mass. at Amherst), B. Schüler (U. Zurich), D. A. Lawrence (U. Chicago), J. Raquena (U. Santiago de Compostela), V.Vento (U. Valencia), S Gosavi (Indian National Centre for Biological Studies).

Patents

1. "A method for identifying intermediates", E. Biasini and P. Faccioli, Identification code: US20210313007, July 2019 (IP share: 50%)
2. "Small molecules inducing degradation of the cellular prion protein", L. Berreca, E. Biasini, and P. Faccioli, WO2021191883, International filing date 29.03.21 (IP share: 30%).

[2]List of past and present *senior* (i.e., PI) collaborators affiliated to foreign institutions and co-authoring at least of my papers.

Summary of Research Activity

Early work in subatomic physics. During the early stage of my career, my research focused on the fundamental theory of strong interaction (Quantum Chromodynamics), mostly addressing the question of how the mass and the electro-magnetic structure of strongly interacting subatomic particles emerges from the dynamical and statistical correlations between their constituents (see, e.g., [1, 8, 9, 23]). This work was carried out within an international network of collaborators including institutes such as MIT, SUNY-Stony Brook, U. Colorado at Boulder, U. Trento, U. Valencia, ECT*, CEA-Saclay, leading to about 30 peer-reviewed publications.

Enhancing macromolecular simulations with theoretical physics. After earning a tenured academic position in subnuclear physics, I shifted the focus of my research toward cross-disciplinary applications of theoretical physics to investigate the dynamics of soft and biological matter. This initiative eventually led to establishing the Statistical and Biological Physics Group within the Physics Department of Trento University, a process that involved hiring three tenured professors [3]. A significant part of my research activity in this field has concerned the development of advanced computational schemes to simulate rare structural re-arrangments of biomolecules, by exploiting and adapting advanced mathematical methods and approximations that had been originally conceived within the context of quantum many-body theory and quantum field theory [28, 30, 51, 55]. We have applied these schemes to simulate large protein conformational changes [50, 65], protein and RNA folding [41, 42, 46, 77], and misfolding [60, 62]. We extensively validated our schemes against ultra-long plain Molecular Dynamics (MD) simulations [41, 51, 66], as well as biophysical experiments and biochemical essays (see, e.g., [57, 53, 68]). Related work concerned adapting renormalization group-based techniques to extract kinetic and thermodynamic information from MD simulations [34, 35, 52, 59]. We derived the $\mathcal{O}(\hbar^2)$ semiclassical correction to the multi-dimensional Fokker-Planck equation and used it to investigate the effects of atomic zero-point quantum fluctuations on the structural dynamics of macromolecules [40]. In another related research direction, we developed a quantum field theory to investigate the real-time propagation of opto-electronic excitations in biomolecules, using both analytic Feynman diagrams methods and numerical stochastic approaches. We applied this theory to molecular wires, amorphous semiconductors, and light-harvesting macromolecular complexes [44, 45, 49, 54, 64].

Since 2020, my research evolved toward developing a new paradigm of macromolecular simulation based on integrating theoretical physics tools with machine learning and quantum computing technologies. Our first applications have ranged from macromolecules' transition path sampling [81, 82, 84], polymer physics [80, 83, 86], to protein design [85]. In a collaboration with Sibylla Biotech S.p.A., we are currently developing and applying quantum computing algorithms for *de-novo* drug design.

Cross-disciplinary applications of enhanced molecular simulations to structural biology and life science. As our algorithms for macromolecular simulations matured, it gradually emerged that we were, for the first time, in the condition of accurately predicting the (re)-folding pathways of *biologically relevant proteins* (i.e., chains consisting of several hundreds of amino acids) using

[3] https://sbp.physics.unitn.it

Figure 1: The official logo of Sibylla Biotech S.p.A. Image taken from www.sibyllabiotech.it.

state-of-the-art atomistic models, given in input the three-dimensional protein native structure. We exploited this technology in a number cross-disciplinary collaborations with several biochemists, molecular, and structural biologists at U. Trento, U. Padua, U. Maryland at Baltimore, U. Santiago de Compostela, U. Illinois. A common factor of all these projects is the use of our enhanced simulation schemes to unveil possible functional, pathogenic, and pharmacological role of protein folding intermediates [76, 62, 69, 73, 78]. In particular, a recent study mapped cryptic phosphorylation sites within the human proteome, revealing that one-third of phosphorylated proteins have sites buried in their interior, which are exposed during the folding process. These cryptic sites, if phosphorylated, could destabilize the protein structure and promote degradation. The findings suggested a crucial role for co-translational phosphorylation in controlling protein folding and stability, with implications for health and disease, as phosphomimetic mutations in these cryptic sites have been linked to increased tumor fitness [79].

Technology Transfer: from Sibylla Biotech S.p.A. to the ZePrion initiative

A new paradigm for rational drug discovery: The possibilty of accurately simulating protein folding pathways at atomic resolution led to conceiving and patenting a completely new protocol for rational drug discovery, named **Pharmacological Protein Inactivation by Folding Intermediates Targeting** (PPI-FIT), co-invented with Prof. E. Biasini, from U. Trento. The rationale underlying this new approach is that targeting a theoretically predicted metastable folding intermediate with small ligands would hinder the folding process, thus promoting protein degradation by the cellular quality control machinery. This scheme was first experimentally validated on the cellular prion protein (PrP), a target involved in several fatal neurodegenerative diseases that is considered undruggable with conventional methods [69].

The development of the PPI-FIT technology led to the founding of **Sibylla Biotech**[4], a research spin-off of INFN, Telethon Foundation, Trento University and Perugia University. Sibylla Biotech is the exclusive licensee of the PPI-FIT patent and operates by developing internal drug discovery pipelines as well as through partnerships with Pharma companies. The innovative character of Sibylla Biotech's PPI-FIT technology led to several international recognitions. In 2019, the company received a first seed investment 2.4 million Eur from venture capital VERTIS SGR. In 2021, it was selected among the 8 world finalists of the "Nature Merck Spin-off Prize". Following up on this, Nature published two articles about the PPI-FIT methodology and its technology transfer

[4] www.sibyllabiotech.it

Figure 2: The official patches of the ZePrion-I and ZePrion-II experiments.

operation[5]. In 2022, Sibylla reached the milestone of 1 million Eur revenues and signed a Series-A investment contract with an international pool of venture capital funds for 23 million Eur. In July 2023, the company relocated from Trento to Bresso (Milan). It now includes 30+ employees, with an international staff, management, and Board of Directors, currently chaired by former CEO of Bayer Pharmaceuticals, Dr. D. Weinand. I have served as chair of Sibylla's Scientific Advisory Board from 2017 through 2021. Since 2021, I am coordinating a scientific partnerships between Sibylla Biotech and U. Milan-Bicocca, aiming at pioneering new computational technologies for drug discovery based on integrating molecular simulations, machine learning, and quantum computing.

The ZePrion Initiative. Our work on physiological, pathological, and pharmacological roles on protein folding intermediates highlighted the importance of obtaining atomically detailed structural information about non-native protein conformations via X-ray crystallography. Unfortunately, obtaining crystals of artificially stabilized non-native protein conformers can be extremely challenging, due to the high aggregation and precipitation propensity of partially folded protein structures. A number of studies have shown that microgravity conditions are ideal for carrying out particularly delicate crystallization processes, due to the absence of convective motions. This observation led to the the ZePrion initiative, an international collaboration involving academic institutions in Milan, Trento, Perugia, Santiago de Compostela, and Marseille, along with multi-national company SpacePharma, a world leader in space-based biomedical technology. ZePrion's scientific endeavour consists of three space missions carried out on the International Space Station (ISS). ZePrion-I was launched in August 2023 and aimed at comparing the aggregation kinetics of partially folded PrP proteins in space and on Earth. Unfortunately, the experimental setup was damaged during the re-entering phase and the data that could be retrieved, although encouraging, were not fully conclusive. The second experiment (ZePrion-II) was launched on August 24th, 2025 and is currently ongoing. Zeprion-II aims at performing zero-gravity crystallization of different native proteins. The key technological advancement involved in ZePrion-II is the design and realization of a fully authomatized lab-in-a-box chip that enables spanning over a matrix of different crystallization conditions, without requiring any astronaut time. ZePrion-II is cofounded by the Euroean Space Organization (ESA) under the BSGN program. Serving as scientific spokesperson of the ZePrion collaboration from 2021 to 2025, I coordinated the collaborative cross-disciplinary work leading to the design and realization of the experimental setups. I signed as PI the successful grant application for ESA support of ZePrion-II. If ZePrion-II will be successful, Zeprion-III will follow, to develop the microgravity technology required to obtain crystallization of partially folded proteins.

[5] "Turning transient structures into drug targets", Nature Outlook: https://www.nature.com/articles/d41586-021-01668-7—

Publications

Theoretical Subnuclear Physics

[1] "Polarized Parton Distributions and Light-Front Dynamics", PF, M. Traini, and V. Vento, Nucl. Phys. A656, 400 (1999).

[2] "Orbital Angular Momentum Parton Distributions and Light Front Dynamics", F. Cano, PF, and M. Traini, Phys. Rev. D62, 054023 (2000).

[3] "Probing Relativistic Spin Effect in the Nucleon by Means of Drell-Yang Processes", F. Cano, PF, and M. Traini, Phys. Rev. D62, 094018 (2000).

[4] "Instanton Contribution to the Proton and Neutron Electric Form Factors", PF, A. Schwenk, and E.V. Shuryak, Phys. Lett. B549, 93(2002).

[5] "A Systematic Study of the Single Instanton Approximation in QCD", PF, and E.V. Shuryak, Phys. Rev. D64, 114020 (2002).

[6] "Proton Electro-magnetic Form Factors in the Instanton Liquid Model", PF and E.V. Shuryak, Phys. Rev. D65, 076002 (2002).

[7] "Parameter-Free Calculation of Hadronic Masses from Instantons", PF, Phys. Rev. D65, 094014 (2002).

[8] "Evidence for Instanton-Induced Dynamics, from Lattice QCD", PF and T.A. DeGrand, Phys. Rev. Lett. 91, 182001(2003).

[9] "Prediction for the Pion Electro-magnetic Formfactor at $Q^2 > 1\text{GeV}^2$ from Instantons", PF, A. Schwenk, and E.V. Shuryak, Phys. Rev. D67, 113009 (2003).

[10] "Instanton Contribution to the Electro-Magnetic Form Factors of the Nucleon", PF, Phys. Rev. C69, 065211(2004).

[11] "Instantons, Diquarks and the $\Delta I = \frac{1}{2}$ Rule for Hyperon Non-Leptonic Weak Decays", M. Cristoforetti, PF, E.V. Shuryak, and M. Traini, Phys. Rev. D70, 054016 (2004).

[12] "The Neutron Electric Dipole Moment in the Instanton Vacuum: Quenched Versus Unquenched Simulations", PF, D. Guadagnoli, and S. Simula, Phys. Rev. D70, 074017(2004).

[13] "Strong CP Breaking and Quark-Antiquark Repulsion in QCD, at Finite θ ", PF Phys. Rev. D71 (Rapid Comm.), 091502 (2005).

[14] "Are There Diquarks in the Nucleon?", M. Cristoforetti, PF, G. Ripka, and M. Traini, Phys. Rev. D 71 114010 (2005).

[15] "Exploring the Chiral Regime of QCD Using the Instanton Liquid Model", M.Cristoforetti, PF, M. Traini and J.W. Negele, Phys. Rev. D75 034008 (2007).

[16] "Instantons Chiral Dynamics and Hadronic Resonances" M.Cristoforetti, PF, and M. Traini, Phys. Rev. D75, 054024(2007).

[17] "Strong CP Violation in External Magnetic Fields", R. Millo and PF, Phys. Rev. D77, 065013 (2008).

[18] "The Scalar Glueball in the Instanton Vacuum", M. Tichy and PF, Europ. Phys. J. C63, 423 (2009).

[19] "CP Violations in Low-Energy Photon-Photon Interactions", R. Millo and PF, Phys. Rev. D79, 065020 (2009) .

[20] "A Path Integral for Heavy Quarks in a Hot Plasma", A. Beraudo, J.P. Blaizot, PF, and G.Garberoglio, Nucl. Phys. A 846, 104(2010).

[21] "Quantum Interaction between Non-Perturbative Vacuum Fields", R. Millo, PF and L. Scorzato, Phys. Rev. D81, 074019(2010).

[22] "Computing the Effective Hamiltonian for Low-Energy Vacuum Gauge Fields", R. Millo and PF, Phys. Rev. D84, 034504(2011).

[23] "QCD Topology at Finite Temperature: Statistical Mechanics of Self-Dual Dyons", PF and E. V. Shuryak, Phys. Rev. D87, 074009 (2013).

[24] "Heavy Quark Bound States in a Quark-Gluon Plasma: Dissociation and Recombination", J.-P. Blaizot, D. De Boni, PF, and G. Garberoglio, Nucl. Phys. A946 49 (2016).

[25] "Effective Field Theory for Quantum Electrodynamics of Graphene Wires", PF and E. Lipparini, Phys. Rev. B80, 045405 (2009).

[26] "The Effect of Interactions on the Conductance of Graphene Nanoribbons", M. Bazzanella, PF and E. Lipparini, Phys. Rev. B82, 1(2010).

[27] "Stochastic Dynamics and Bound States of Heavy Impurities in a Fermi Bath", M. Sighinolfi, D. De Boni, A. Roggero, G. Garberoglio, PF, and A. Recati, Phys. Rev. A 105, 043308 (2022).

Statistical and Biological Physics, Life Science, and Drug Discovery

[28] "Dominant Protein Folding Pathways", PF, M. Sega, F. Pederiva, and H. Orland, Phys. Rev. Lett. 97, 108101(2006).

[29] "Molecular Dynamics Simulations Suggests Possible Interaction Patterns at Early Steps of β_2-microglobulin aggregation", F.Fogolari, A. Corazza, P. Viglino, P. Zuccato, L. Pieri, PF, V. Bellotti, and G. Esposito, Biophys. J. BioFAST: doi:10.1529/biophysj.106.098483 (2006).

[30] "Quantitative Protein Dynamics from Dominant Folding Pathways", M.Sega, PF, F. Pederiva, G. Garberoglio, and H. Orland, Phys. Rev. Lett. 99, 118102 (2007).

[31] "Characterization of Protein Folding from Dominant Reaction Pathways" PF, J. Phys. Chem. B112, 13756 (2008).

[32] "Stochastic Dynamics and Dominant Protein Folding Pathways", PF, M. Sega, F. Pederiva, and H. Orland, Phil. Mag. 88., 4093 (2008).

[33] "Dominant Reaction Pathways in High Dimensional Systems", E. Autieri, PF, M. Sega, F. Pederiva, and H. Orland, , J. Chem. Phys. 130 064106 (2009).

[34] "Simulating Stochastic Dynamics Using Large Time Steps", O. Corradini, PF, and H. Orland, Phys. Rev. E80, 061112 (2009).

[35] "Molecular Dynamics at Low Time Resolution", PF, J. Chem. Phys. 133, 164106 (2010).

[36] "Dominant Pathways in Protein Folding: a Direct Validation Against MD Simulations", PF, A. Lonardi, and H.Orland, J. Chem. Phys. 133, 045104 (2010).

[37] "Communications:Ab-initio Dynamics of Rare Thermally Activated Reactions", S. a Beccara, G. Garberoglio, PF, and F. Pederiva, J. Chem. Phys. 132, 111102 (2010).

[38] "Fluctuations in the Ensemble of Reaction Pathways", G. Mazzola, S. a Beccara, PF, and H. Orland, J. Chem. Phys. 134, 164109 (2011).

[39] "Dominant Folding Pathways of a Peptide Chain, from Ab-Initio Quantum-Mechanical Simulations", S. a Beccara, PF, G. Garberoglio, M. Sega, F. Pederiva, and H. Orland, J. Chem. Phys. 134024501 (2011) (selected as journal cover).

[40] "Quantum Diffusive Dynamics of Macro-molecular Transitions", S. a Beccara, PF, and G. Garberoglio, J. Chem. Phys. 136, 214111 (2012).

[41] "Dominant Folding Pathways of a WW Domain", S. a Beccara, T. Skrbic, R. Covino, and PF, Proc. Natl. Acad. Sci. U.S.A. 1092330 (2012).

[42] "The Role of Non-Native Interactions in the Folding of Knotted Proteins", T. Skrbic, C. Micheletti, and PF, PLoS Comp. Biol. 8 e1002504 (2012)

[43] "Microscopically Computing Free-energy Profiles and Transition Path Time of Rare Macromolecular Transitions", PF and F. Pederiva, Phys. Rev. E. 86, 061916 (2012).

[44] "Quantum Charge Transport and Conformational Dynamics of Macromolecules", L. Boninsegna and PF, J. Chem. Phys. 136, 214111 (2012).

[45] "Dissipative Quantum Transport in Macromolecules: An Effective Field Theory Approach", E. Schneider, S. a Beccara, and PF, Phys. Rev. B88, 085428 (2013).

[46] "Folding of a Knotted Protein From with a Realistic All Atom Force Field", T. Skrbic, S. a Beccara, R. Covino, C. Micheletti, and PF, PLoS Comp. Biol. 9, e1003002 (2013).

[47] "Unfolding Thermodynamics and Molecular Adaptation of Cystein-Rich Proteins", G. Cazzolli, T. Skrbic, G. Guella, and PF, Biomolecules 3, 967 (2013).

[48] "The Role of Non-Native Interactions in the Folding of Knotted Proteins: Insights from Molecular Dynamics Simulations", R. Covino, T. Skrbic, PF, C. Micheletti, Biomolecules 4, 1 (2013).

[49] "Long-Distance Quantum Transport Dynamics in Macromolecules", E. Schneider and PF, Phys. Rev. B89, 134305 (2014).

[50] "Serpin Latency Transition at Atomic Resolution", G. Cazzolli, F. Wang, S. a Beccara, A Gershenson, PF, P. Wintrode, Proc. Natl. Acad. Sci. U.S.A. 111,15414 (2014).

[51] "Variational Scheme to Compute Protein Reaction Pathways Using Atomistic Force Fields with Explicit Solvent", S. a Beccara, L. Fant, and PF, Phys. Rev. Lett. 114, 098103 (2015).

[52] "Dimensional Reduction of Markov State Models from Renormalization Group Theory", S. Orioli, and PF, J. Chem. Phys. 145, 124120 (2016).

[53] "Folding Mechanism of Proteins Im7 and Im9: Insight from All-Atom Simulations in Implicit and Explicit Solvent", F. Wang, G. Cazzolli, P. Wintrode, and PF, J. Phys. Chem. B120, 9297 (2016).

[54] "Quantum Propagation of Electronic Excitations in Macromolecules: A Computationally Efficient Multiscale Approach", E. Schneider, S. a Beccara, F. Mascherpa, and PF, Phys. Rev. B94, 014306 (2016)

[55] "Self-Consistent Calculation of Protein Folding Pathways", S. Orioli, S. a. Beccara, and PF, J. Chem. Phys. 147, 064108 (2017).

[56] "All-atom Calculation of Protein Free-Energy Profiles", S. Orioli, A. Ianeselli, G. Spagnolli, and PF, J. Chem. Phys. 147, 152724 (2017).

[57] "The Atomic Detail of Protein Folding Revealed by an Ab-Initio Reappraisal of Circular Dichroism", A. Ianeselli, S. Orioli, G. Spagnolli, PF, L. Cupellini, S. Jurinovich, and B. Mennucci, JACS 140, 3674 (2018). -co-corr. author-.

[58] "Predicting Charge Mobility in Organic Semiconductors with Complex Morphology", F. Segatta, G. Lattanzi and PF, Macromolecules 51, 9060 (2018)

[59] "Transition Path Theory from Biased Simulations", G. Bartolucci, S. Orioli, and PF, J. Chem. Phys. 149, 072336 (2018).

[60] "All-Atom Simulations Reveal How Single Point Mutations Promote Serpin Misfolding", F. Wang, S. Orioli, A. Ianeselli, G. Spagnolli, S. a Beccara, A. Gershenson, PF, and P. L. Wintrode, Biophys. J. 114 2083 (2018).

[61] "Allostery in its Many Disguises: From Theory to Applications" SJ Wodak et al. Structure 10 (2019).

[62] "Full Atomistic Model of Prion Structure and Conversion", G. Spagnolli, M. Rigoli, S. Orioli, A. M. Sevillano, PF, H. Wille, E. Biasini, J. R. Requena, PLoS Pathog 15: e1007864 (2019).

[63] "Ok Google, How Could i Design Therapeutics Against Prion Diseases?" M Rigoli, G Spagnolli, PF, JR Requena, E Biasini Curr. Opin. in Pharmacology 44, 39-45 (2019).

[64] "Microscopic Calculation of Absorption Spectra of Macromolecules: an Analytic Approach" M Carli, M Turelli, and PF J. Chem. Phys 150 (14), 14410 (2019).

[65] "The Molecular Mechanisms of Photo-activation of Orange Carotenoid Protein Revealed by Molecular Dynamics", M. Bondanza, L. Cupellini, PF, and B. Mennucci. JACS 142, 21829 (2020).

[66] "All-Atom Simulation of HET-s Prion Replication", L. Terruzzi, G. Spagnolli, A. Boldrini, J. R. Requena, E. Biasini, and PF, PLoS Comput Biol 16(9) : e1007922 (2020).

[67] "Successes and Challenges in Simulating the Folding of Large Proteins", A. Gershenson, S. Gosavi, PF, and P.L. Wintrode, J. Biol. Chem. 295, 15 (2020).

[68] "Slow Escape from a Helical Misfolded State of the Pore-Forming toxin Cytolysin A", F. Dingfelder, I. Macocco, S. Benke, D. Nettels, PF, and B. Schüler, JACS Au 1, 1217 (2021) - co-corr. author-.

[69] "Pharmacological Inactivation of the Prion Protein by Targeting a Folding Intermediateby", G. Spagnolli et al. Comms. Biol. (Nature PG) 462 (2021) - co-corr. author-.

[70] "Target Search of Active Agents Crossing High Energy Barriers", L. Zanovello, M. Caraglio, T. Franosh, and PF, Phys. Rev. Lett. 126, 018001 (2021).

[71] "Optimal Navigation Strategy of Active Brownian Particles in Target-Search Problems", L. Zanovello, PF, T. Franosch, and M. Caraglio, J. Chem. Phys. 155, 084901 (2021).

[72] "How Theoretical Nuclear Physics Can Help Discover New Drugs", PF Nucl. Phys. News. 31 (1), 29 (2021).

[73] "Long range allostery mediates the regulation of plasminogen activator inhibitor-1 by cell adhesion factor vitronectin" , K. Kihn, E. Marchiori, G. Spagnolli, A. Boldrini, L. Terruzzi, D. A. Lawrence, A. Gershenson, PF , and P. L. Wintrode, J. Biol. Chem. 298, 102652 (2022).

[74] "Computer-aided comprehensive explorations of RNA structural polymorphism through complementary simulation methods", K. Röder, G. Stinermann, PF, and S. Pasquali, QRB Discovery, 3: e21 (2022).

[75] "Survival Strategies of Artificial Active Agents" L. Zanovello, R.J.G. Löffler, M Caraglio, T. Franosch, M.M. Hanczyc, PF Scientific Reports 13 (1), 5616 (2023).

[76] "Functional, pathogenic, and pharmacological roles of protein folding intermediates" E Biasini, PF, Proteins: Structure, Function, and Bioinformatics (2023) doi.org/10.1002/prot.26479.

[77] "RNA Folding Pathways from All-Atom Simulations with a Variationally Improved History-Dependent Bias", G. Lazzeri, C. Micheletti, S. Pasquali, and PF, Biophysical J. 122, 3089 (2023).

[78] "The Evolution of Eukaryotic Linear Motifs Governing the Function of Androgen Receptor from Fish to Homo Sapiens", A. Falconieri *et al.*, Nucleic Acid Research, 53, gkaf688 (2025).

[79] "Mapping Cryptic Phosphorylation Sites in the Human Proteome", D. Gasparotto *et al.*, EMBO J., in press (2025).

Integrated Applications of Quantum Computing and Machine Learning to Molecular Simulations

[80] "Polymer Physics by Quantum Computing", C. Micheletti, P. Hauke, and PF, Phys. Rev. Lett. 127, 080501 (2021).

[81] "Dominant Reaction Pathways by Quantum Computing", P. Hauke, G. Mattiotti, and PF, Phys. Rev. Lett.126, 028104 (2021).

[82] "Sampling Rare Conformational Transitions with a Quantum Computer", D. Ghamari, P. Hauke, R. Covino, and PF, Scientific Reports 12, 16336 (2022).

[83] "Quantum-inspired Encoding Enhances Stochastic Sampling of Soft Matter Systems", F. Slongo, P. Hauke, PF, and C. Micheletti, Science Advances 9, eadi0204 (2023).

[84] "Sampling a Rare Protein Transition Using Quantum Annealing", D. Ghamari, R. Covino, and PF, JCTC 20 (8), 3322-3334 (2024).

[85] "Protein Design by Integrating Machine Learning and Quantum-Encoded Optimization", V Panizza, P Hauke, C Micheletti, and PF, PRX Life 2 (4), 043012 (2024).

[86] "Statistical Mechanics of Heteropolymers from Lattice Gauge Theory", V. Panizza, A. Roggero, P. Hauke, and PF, Phys. Rev. Lett. 134 (15), 158101 (2025). (Editor's suggestion.)