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Editorial

Physchem: A New Physical Chemistry Journal

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Physical chemistry is broadly defined as the branch of chemistry devoted to the study of how matter behaves on a molecular and atomic level and how chemical reactions occur. G. N. Lewis said "Physical chemistry is everything that is interesting and exciting!" While there are many different definitions of the discipline, it is characterized by the use of physical theory, models and methods in the study of chemistry. The discipline is defined by its approach, rather than by the nature of the systems studied—a stark contrast to the other chemistry disciplines.

The key for understanding human evolution and its impact on our planet might be found in the exploration of the evolution of simple systems towards living cells. This, however, takes us back to the origin of everything, to the fascinating topic of the origin of the solar system, of our planet and of life. In our universe, we witness an extraordinary evolution, from simplicity toward the extraordinary complexity: from the lightest atoms to small molecules, to the building blocks of biomolecules, to living beings and to their interaction with the environment. A physical chemical approach offers a unified framework to understand and rationalize this long journey. We welcome papers which address these phenomena from the physical chemistry viewpoint.

Climate, environment and their changes caused by anthropogenic activities have becomecentral topics in fundamental and applied research and, due to the perceived rapid pace of the climate and environmental modifications, the need for news technologic solutions as well as new competences and professional figures will rapidly grow in the next future. For example, population growth is putting high demand on our energy and chemical supply chains, demanding novel and sustainable approaches for the production of clean electricity, fuels and chemicals. Photovoltaics, batteries and catalysis are central for a sustainable production and storage of renewable energy. Those systems range from natural to artificial and cover the catalysis field longitudinally. We welcome papers dedicated to the understanding those systems, as well as studies guiding the development subsequent generations of systems.

Nanoscience, the study of structures and materials on an ultra-small scale, has the potential to revolutionize a wide range of fields, from health care to manufacturing. At the nanometer level, the physical and chemical properties of matter change, which affects their chemical reactivity, thermodynamic, surface and interface compositions and interactions. We welcome articles generating insights into the nanoworld, including nanomaterials properties, interactions and reactivity, as well as novel spectroscopic, diffraction and imaging methodologies.

The two historical pillars of physical chemistry are theory and experiment. More recently, computer-based simulations have provided a third well-established pillar, which is being further strengthened by the ongoing improvement of software and increase of computer power, with quantum computing paving the route for a new revolution in this field. Computer modeling and simulation have been increasing in importance when solving problems in physical chemistry. Computations assist in the discovery and rational design of

Citation: Barone, V.; Manzhos, S.; Sá, J. PhysChem: A New Physical Chemistry Journal. *Physchem* **2021**, *1*, 1–3. https://dx.doi.org/10.3390/physchem1010001

Received: 26 November 2020
Accepted: 27 November 2020
Published: 14 December 2020

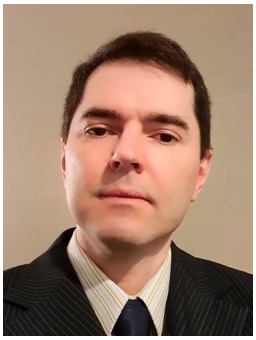
materials for various technologies. They can provide mechanistic insight otherwise not directly accessible with experiments, which can assist in rational design of materials for novel types of batteries, solar cells, alloys, etc. They can help prescreen materials before expensive experimentation begins and then explain experimental results. We especially welcome manuscripts dealing with novel or improved theoretical frameworks and experimental techniques, which are needed on one hand to improve conceptual understanding of matter and phenomena, and on the other to improve modeling capabilities thereof. We also look forward to submissions proposing theoretical developments and computational methods allowing for more accurate modeling: this includes methods aimed at accurate modeling at large (more realistic) time and length scales.

An important emergent type of approaches that help solve problems in physical chemistry and chemical physics are machine learning (ML) and artificial intelligence (AI) based approaches. Recent years have seen an explosion of literature applying ML approaches to all sorts of problems, including those in the domain of physical chemistry: functional developments for DFT, the construction of interatomic potentials, Δ-learning used to boost the accuracy of known simulation methods, etc. This trend is set to continue. In parallel, virtual reality and augmented reality (VR/AR) are revolutionary tools that allow for creating interpretable visualizations to study complex data, with exploration and analysis being enhanced by one's own perceptive and proprioceptive system. The combination of AI and VR/AR will allow both experimentally- and computationally-oriented researchers to automatically perform all the steps required for the design and analysis of new experiments and to select the most effective integrated strategy. We are especially looking forward to submissions applying AI techniques, properly speaking (i.e., artificial reasoning as opposed to regression/classification), to problems in physical chemistry and papers developing novel ML- and AI-based methods specifically for such problems. We also welcome papers devoted to the description of ongoing efforts toward the development of the different pieces of this complex framework in which experimental, computational, data and visualization components will be connected to people by software, with the aim of improving research throughput and achieving goals which are otherwise not possible.

Conflicts of Interest: The authors declare no conflict of interest.

Short Biography of Authors

Vincenzo Barone has been a full professor of physical chemistry since 1994: first at the Federico II University, Naples, Italy, and then, since 2008, at the Scuola Normale Superiore, Pisa, Italy, where he has also been the President from 2016 to 2019. He is a member of several editorial boards, and a fellow of the Accademia Nazionale dei Lincei, the International Academy of Quantum Molecular Sciences, the European Academy of Sciences and the Royal Society of Chemistry. He has been the President of the Italian Chemical Society and has received several national and international prizes and grants (e.g., the Avogadro Medal in 2020, the French–Italian Chemistry prize in 2019 and the ERC Advanced Grant DREAMS in 2013). He has authored more than 800 papers in international journals, with more than 60,000 total citations and an H-index of 90. Since 1995, he has been one of the major contributors of the Gaussian package, which is the most widespread electronic structure code and receives thousands of citations per year. His scientific activity has provided fundamental contributions in fields including density functional theory, solvent models, computational spectroscopy, astrochemistry and also, in the last few years, applications of virtual reality and artificial intelligence to molecular sciences.



Sergei Manzhos is Associate Professor at the Centre Énergie Matériaux Télécommunications (EMT) of the Institut National de la Recherche Scientifique (INRS), Canada. He holds a Ph.D. in chemistry from Queen's University (2005) and M.Sc. in radio physics from Kharkiv National University (1999). In 2004–2008, he was a postdoctoral fellow and NSERC postdoctoral fellow at the Université de Montréal in the group of Prof. Tucker Carrington. He was a Project Assistant Professor at the University of Tokyo (Department of Chemical System Engineering and Research Centre for Advanced Science and Technology) in 2008–2012, working in the group of Prof. Koichi Yamashina and Prof. Hiroshi Segawa. In 2012–2019, he was an Assistant Professor (group leader) at the Department of Mechanical Engineering, National University of Singapore, Singapore, before joining INRS in 2019. Prof. Manzhos's research interests include computational modeling and design of materials for energy conversion and storage technologies, as well as method development for computational spectroscopy and large-scale ab initio methods. He uses and develops machine learning based methods for these and other applications.

Jacinto Sá (Ph.D.-Physical-Chemistry) is the leader of the Plasmonics research group and physical chemistry professor at Uppsala University (Sweden) and Institute of Physical-Chemistry, Polish Academy of Sciences (IChF-PAN), Poland. He attained his MSc in the chemistry field of Analytical Chemistry at the Universidade de Aveiro, Portugal, during which he did a research project at Vienna, University of Technology, Austria. He was awarded a PhD degree in 2007 by the University of Aberdeen, Scotland, UK, in the field of catalysis and surface science. In 2007, he joined as a postdoc the CenTACat group at Queen's University Belfast under the guidance of Profs. Burch and Hardacre. In 2010, he moved to Switzerland as a scientist first at ETH Zurich and Paul Scherrer Institute, and later at the Laboratory for Ultrafast Spectroscopy (EPFL). In 2013, he was awarded by Uppsala University a tenure-track assistant professor, a position competed for by 800 candidates. In 2014, he started the position jointly at Uppsala University and IChF-PAN. He was promoted to full professor in 2020. In 2018, Prof. Sá co-founded Peafowl Solar Power as a start-up, that develops aesthetic power solutions for smart devices based on direct plasmonic solar cells, a concept pioneered in his research group. His research efforts are focused on plasmonic for artificial photosynthesis and solar cells, as well as the development of advanced characterization techniques in particular core-level photon-in photon-out spectroscopy with von Hamos spectrometer from lab to XFEL measurements for a plethora of applications.