MSDE

EDITORIAL

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View Journal

Cite this: DOI: 10.1039/d6me90009g

Introduction to a Festschrift in honour of Juan de Pablo's 60th birthday

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DOI: 10.1039/d6me90009g

rsc.li/molecular-engineering

The joint Royal Society of Chemistry (RSC) and the Institution of Chemical Engineers (IChemE) journal *Molecular Systems Design & Engineering* (*MSDE*) was launched in May 2016 as a venue for research "following the journey from molecular-level design and optimisation through systems-level functionality to real-world applications" and employing "a problem solving strategy or vision based on molecular-level design or optimisation (be it through theory, modelling or experiment) leading to desired systems-level functionality and performance". The vision and leadership of the inaugural Editor-in-Chief Juan de Pablo was instrumental in realizing the journal, and, over the course of his seven-year tenure through to May 2023, raising the journal to an established and respected multidisciplinary venue for the dissemination of novel methods for the design of a broad range of molecules, materials, and molecular systems, and of their application to the discovery and engineering of new chemical, biochemical, and physicochemical systems. We are delighted to present, on the occasion of Juan's 60th birthday, this Festschrift celebrating his scientific accomplishments and commemorating his contributions to *MSDE*.

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Juan was born and raised in Mexico City. He completed a bachelor's degree in chemical engineering at the Universidad Nacional Autónoma de México in 1985, before earning a PhD in chemical engineering at the University of California, Berkeley, in 1990 under the supervision of John Prausnitz. He then completed postdoctoral training at the Swiss Federal Institute of Technology in Zurich, Switzerland, before establishing an independent research group as a new faculty member at the University of Wisconsin – Madison in 1992, where he rose through the ranks to ultimately serve as the Howard Curler Distinguished Professor and Hilldale Professor of Chemical Engineering. In 2012, he joined the newly established Institute for Molecular Engineering at the University of Chicago, which subsequently became the Pritzker School of Molecular Engineering, as a founding faculty member and Liew Family Professor of Molecular Engineering and Senior Scientist at Argonne National Laboratory. During his time at the University of Chicago, he took on a number of senior institutional leadership roles, including an appointment as the Vice President for National Laboratories, Science Strategy, Innovation and Global Initiatives, and Executive Vice President for Science, Innovation, National Laboratories and Global Initiatives. In 2024, he moved to New York University, where he was appointed the inaugural Executive Vice President for Global Science and Technology and the Executive Dean of the Tandon School of Engineering.

Juan is a prominent and prolific researcher with broad interests in materials science and chemical engineering who has co-authored over 600 scientific publications. He maintains a vibrant research portfolio focused on molecular modeling and simulation of polymers, biomolecules, glasses, and liquid crystals. He is well known for his development of advanced computer simulation methods to understand and engineer molecules and materials by combining tools from statistical thermodynamics, numerical methods, machine learning, and multi-scale modeling. Some of Juan's noted accomplishments include development of the expanded density of states (EXEDOS) algorithm, discovery of potential vulnerabilities in the SARS-CoV-2 proteins, methods to control the motion of topological defects in liquid crystals, and development of block copolymer directed self-assembly techniques to create nanoscale patterns for semiconductor manufacturing. For these achievements, among many more, Juan has been recognized by numerous awards and honors including the 2011 Charles Stine Award from the American Institute of Chemical Engineers, the 2016 DuPont Medal for excellence in nutrition and health science, and the 2018 American Physical Society Polymer Physics Prize. He is a fellow of the American Academy of Arts and Sciences,

the American Physical Society and an honorary member of the Mexican Academy of Sciences, and was inducted into the US National Academy of Engineering in 2016 and the US National Academy of Sciences in 2022. He holds more than 25 patents and is the co-author of the textbook *Molecular Engineering Thermodynamics* (2011).

The 24 articles from Juan's collaborators, students, and friends collected in this Festschrift encompass a variety of topics in molecular and materials science and engineering. The range of topics, spanning both methods and applications, is a testament to Juan's diverse scientific interests and his broad influence as a mentor and collaborator. Given Juan's seminal contributions to polymer research, the collection contains some wide-ranging studies of this class of materials, including a self-consistent field study of the phase behavior of pentablock copolymer melts led by Arthi Jayaraman (https://doi.org/10.1039/D4ME00138A), a free-energy study of adsorption in flexible soft coordination polymers by led by Yamil Colón (https://doi.org/10.1039/D4ME00154K), multi-scale modeling of polymer adhesion led by Doros Theodorou (https://doi.org/10.1039/D4ME00199K), or the design of shape morphing liquid-crystal elastomers led by Rui Zhang (https://doi.org/10.1039/D5ME00046G). The article collection also offers an opportunity to explore the phase behavior and design of emerging materials through a critical review of simulation methods for intrinsically disordered proteins led by Jeffery Saven and Kristi Kiick (https://doi.org/10.1039/D4ME00197D), a combined microfluidic/continuum simulation study of the effect of confinement on the structure of cholesteric liquid crystals led by Monirosadat Sadati (https://doi.org/10.1039/D5ME00070J), or a predictive method to support the development of antibody crystallization methods led by Bernhardt Trout (https://doi.org/10.1039/D4ME00187G). As is fitting for *MSDE*, methods that support the rapid discovery of novel materials and their properties feature prominently in these articles as well as in the bio-inspired approach to the design of water-responsive nanocomposite materials proposed by LaShanda Korley and co-authors (https://doi.org/10.1039/D4ME00177J), the toolkit of Marc-Olivier Coppens and co-authors for the design of 3D Voronoi structures (https://doi.org/10.1039/D4ME00036F), the high-performance classifier for enzymatic reactions proposed by a team led by Keith Tyo (https://doi.org/10.1039/D4ME00118D), the accelerated approach to select suitable parameters for the field-theoretic simulations of complex multicomponent systems from the team of Joshua Lequieu (https://doi.org/10.1039/D5ME00100E), or the rapid prediction of phase diagrams enabled by a physics-informed neural network developed by Michael Webb and collaborators (https://doi.org/10.1039/D4ME00168K). The collection highlights several applications of molecular engineering to address global sustainability challenges, such as the machine-learning-enabled screening of a vast array of metal–organic frameworks (MOFs) for hydrogen storage led by Randall Snurr (https://doi.org/10.1039/D5ME00078E), an exploration of nanostructured ion conductors for lithium-ion batteries led by Takashi Kato (https://doi.org/10.1039/D4ME00176A), and an approach to design probe materials for chemical sensors that can be applied to the detection of PFAS jointly led by Claire Donnat, Yuxin Chen and Junhong Chen (https://doi.org/10.1039/D4ME00203B).

We hope that the readers of *MSDE* enjoy this special collection in celebration of our inaugural Editor-in-Chief and wish Juan all the best on the occasion of his 60th birthday.