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New Editor-in-Chief and Deputy Editor-in-Chief for *MSDE*: reflections and vision

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The first issue of *Molecular Systems Design & Engineering* (*MSDE*) was published in May 2016 as a joint venture between the Royal Society of Chemistry (RSC) and the Institution of Chemical Engineers (IChemE) under Editor-in-Chief Juan de Pablo. On June 1, 2023, we were pleased to be invested as the new Editor-in-Chief and Deputy Editor-in-Chief of the journal (<https://t.co/jyeq5a7lYd>). We have both had the great privilege to work as *MSDE* Editorial Board members over the last few years and to see the journal go from strength to strength and are excited to lead this unique journal into the next phase of its development. Any change in leadership presents an opportunity to reflect upon the progress of the journal and its future evolution, and we are pleased to use this editorial to articulate our vision for the journal and solicit response and feedback from the *MSDE* community.

MSDE was launched with a broad vision to attract and publish work “following the journey from molecular-level design and optimisation through systems level functionality to real-world applications” and employ “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”. Under the leadership of Juan de Pablo, *MSDE* has pursued this vision to become a flagship multidisciplinary journal 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.

Today, the *MSDE* proposition – standing at the crossroads between pressing societal needs and emerging scientific innovation – is ever more timely. *MSDE* authors employ experimental, theoretical and computational approaches to establish new understanding of molecular properties and behaviours, and use this understanding to design and assemble better materials, systems, and processes to achieve specific functions. There is no doubt that new paradigms for molecular and materials design and engineering are urgently needed to make human activity more effective and sustainable. Although this presents a considerable challenge, we are witnessing the convergence of scientific advances that can be brought to bear on the design of multiscale systems spanning from atoms and molecules to products, devices, and manufacturing processes. These trends are being driven by unprecedented new capabilities to characterise molecules and materials at

the nanoscale, conduct high throughput screening, deploy ever more accurate and sophisticated physics-based and data-driven models, train new machine learning models to understand and engineer molecules and materials, and integrate artificial intelligence and automated robotics within “self-driving laboratories”. These powerful tools have enabled the community to make new headway in grand challenges in science and engineering, many of which are closely aligned with UN Sustainable Development Goals. By way of example, in the last few years, *MSDE* readers have been able to discover work employing state-of-the-art techniques to contribute to UNSDG challenges such as clean water and sanitation (<https://doi.org/10.1039/D2ME00284A>), affordable and clean energy (<https://doi.org/10.1039/C9ME00166B>), climate action (<https://doi.org/10.1039/D2ME00130F>) and human health and well-being (<https://doi.org/10.1039/D3ME00059A>).

It is our ambition for *MSDE* to provide a forum to disseminate scientific advances that will translate into solutions to societal challenges, and to enable such advances by supporting a burgeoning multi-disciplinary community of researchers. The combination, within *MSDE*, of articles focused on new methods with those focused on specific applications provides an ideal opportunity to identify cross-pollination between these two distinct, but mutually reinforcing, thrusts: progress in important

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and reader surveys. It is our honour to build upon the achievements of the journal over the first seven years of its life and to work with the editorial staff and the scientific community to steward it towards future success.



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The ability to bring together researchers from often disconnected areas to strengthen the emerging

