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The decade of artificial intelligence in chemistry and materials

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Digital Discovery celebrates its first anniversary. I believe that its launch was timed to perfection and there are two main pieces of evidence to back this up. Firstly, the group of exciting scientific articles on our pages is a corpus that reflects a growing field of activity, both in fundamental new propositions of methods and platforms and an increasingly more extensive set of applications in new molecules, materials, composites and devices. Secondly, and in a broader sense, advances in artificial intelligence (AI) are generally moving at an astonishing pace. This year saw the commoditization of large language models such as GPT-3 (ref. 1) *via* tools like ChatGPT[2] and extremely impressive image generation tools such as Stable Diffusion,[3] and my personal favourite, the recent incredible achievement of a chat-based AI system that plays the game Diplomacy.[4] The field is advancing so quickly that one requires AI to predict the future of AI research[5]!

In its first year, *Digital Discovery* published 95 articles authored by researchers from 22 different countries and covering the breadth of the journal's scope. It would be impossible to describe all the exciting progress reported on our pages. Still, I will select a few works to exemplify the variety of ways the community is building this interdisciplinary field.

For example, in *Digital Discovery* Hocky and White[6] explore the frontiers of automated code generation and how it could affect field practitioners. This study belongs to the cadre of work that represents the tip of the iceberg of what large language models can do for chemistry.

Another exciting advance reported on our pages is the work of Kraus and co-workers.[7] Their team reports on their progress in developing an open framework for *in operando* catalysis measurements. This work exemplifies how the closed-loop characterization of chemical processes can lead to further accelerated progress in discovering functional compositions and conditions for chemical processes. Along the same lines, the elegant work of Sagmeister and co-workers[8] shows how spectra obtained from real-time processes can be translated into useful concentrations. The continued development of AI and automation techniques for characterization will be critical for realizing self-driving laboratories (SDLs).

Our pages contain beautiful examples of closed-loop demonstrations of SDLs for complex and challenging materials optimization goals. For example, Rooney and co-workers report an end-to-end platform for the design of adhesive formulations.[9] Vaddi *et al.*[10] report a comprehensive SDL for the inverse design of gold nanoparticles based on their spectral properties. Closer to applications that could have an incredible impact on climate change, Zhang and co-workers report the automated academic closed-loop assembly and optimization of battery cells on our pages.[11] Concrete is a significant contributor to carbon emissions. Optimizing processes in this incumbent industry with AI is a hot emerging topic. In *Digital Discovery*, Sergis and Ouellet-Plamondon[12] demonstrate the automation and optimization of 3D-printed concrete mixes.

Finally, the field of Bayesian optimization has ample representation on our pages. A couple of examples of work in the area reported this year include the elegant combination of autoencoders and Bayesian optimizers by Valetti and co-workers.[13] They show how to use VAEs as efficient dimensionality reduction tools for Bayesian optimization of experimental or computational trajectories. From our lab, we report Bayesian optimization in chemical settings where known design or experimental constraints are present.[14] This situation is ubiquitous in all SDLs, and we believe the tool will help make more rapid progress in the field.

We continue to innovate in the field by promoting new article types; we

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introduced the **Tutorial Review** article class that allows for authoritative reviews of techniques, methods, or software tools. This article class will help develop this rapidly-developing field, eliminating the constraints of rigid article types. We are looking to include more article types in the future to allow the publication of the variety of outputs produced by researchers working in the field.

We celebrated the success of the Accelerate Conference held in Toronto in the Fall of last year as a landmark for the field. The journal was a supporter of the conference. We hope to continue working together so that the area has opportunities to interact digitally or in person.

I look forward to 2023 as a cornerstone year for this journal and the field at large. May all the journal authors and readers have a wonderful new year.

Alán Aspuru-Guzik, Editor in Chief

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