

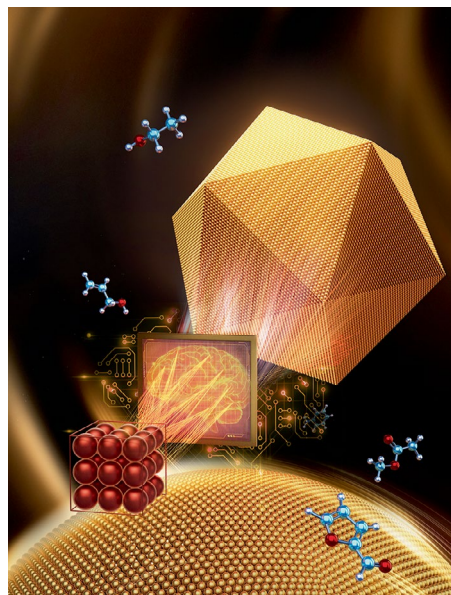
# Cover runners-up of 2025

 Check for updates

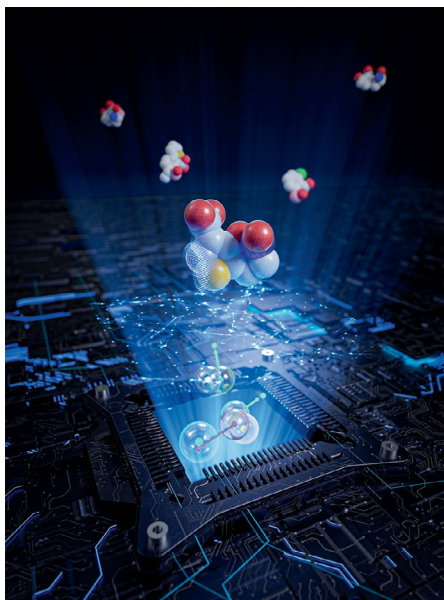
We highlight some of our favorite cover suggestions from 2025.

**W**e continue our yearly tradition of highlighting our favorite author-suggested covers that were not chosen as *Nature Computational Science* covers.

The first image was submitted by Xiaonan Wang and colleagues for their paper on a model – named SurFF – for predicting catalyst surface exposure from bulk crystal structures at scale<sup>1</sup>. The red-sphere cubic lattice in the lower left represents the bulk intermetallic crystal (unit cell) used as the starting input. From this bulk structure, SurFF evaluates many possible surface terminations/facets and learns facet-dependent energetics with a machine-learning force field, which is depicted in the image by the chip with a brain icon and surrounding circuit traces. The radiating light/streams indicate high-throughput inference from the learned model to the materials output. The predicted surface energetics are then translated into a Wulff construction



Cover submitted for the paper by Xiaonan Wang and colleagues. Credit: Jun Yin and Xiaonan Wang.



Cover submitted for the paper by Guo-Bo Li and colleagues. Credit: Guo-Bo Li and Jian Peng.

(a method for predicting the equilibrium shape of nanoparticles), visualized as the large gold polyhedral nanoparticle, whose facet sizes correspond to the thermodynamically preferred surface area fractions. The metal atomic surface at the bottom of the image illustrates the resulting exposed facets as physically meaningful catalytic interfaces, while the surrounding small molecules represent reactants/intermediates interacting with the predicted surfaces.

Another cover runner-up was submitted by Guo-Bo Li and colleagues for their paper on a computational model – termed Phore-Gen – that facilitates the identification of pharmacophore features and the generation of corresponding new small molecules<sup>2</sup>. The integrated circuit symbolizes the deep learning framework, acting as the computational engine driving the design process. Luminous spheres emerge from the chip, representing various pharmacophore features, while three-dimensional molecules aligning with these features are generated, highlighting pharmacophore-guided molecular design. The beam of light represents the



Cover submitted for the paper by Kevin Maik Jablonka and colleagues. Credit: Indrajeet Mandal.

diffusion-denoising process, illustrating how the model transforms noise into precise, chemically valid molecules.

Last but not least, an image submitted for the paper by Kevin Maik Jablonka and colleagues is also worth highlighting<sup>3</sup>. The figure depicts a luminous wireframe hand – which represents artificial intelligence, and more specifically, a vision language models (VLM) – writing on a laboratory notebook filled with notes related to chemistry and materials science. Here, the act of writing represents active scientific thinking, interpretation of experimental data, and formation of meaningful conclusions. The paper introduces a benchmark – named MaCBench – to evaluate whether modern VLMs can truly reason across chemistry and materials science like a scientist, or merely recognize patterns.

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## References

1. Yin, J. et al. *Nat. Comput. Sci.* **5**, 782–792 (2025).
2. Peng, J. et al. *Nat. Comput. Sci.* **5**, 898–914 (2025).
3. Alampara, N. et al. *Nat. Comput. Sci.* **5**, 952–961 (2025).