Success Stories in Chemical Sciences & Materials

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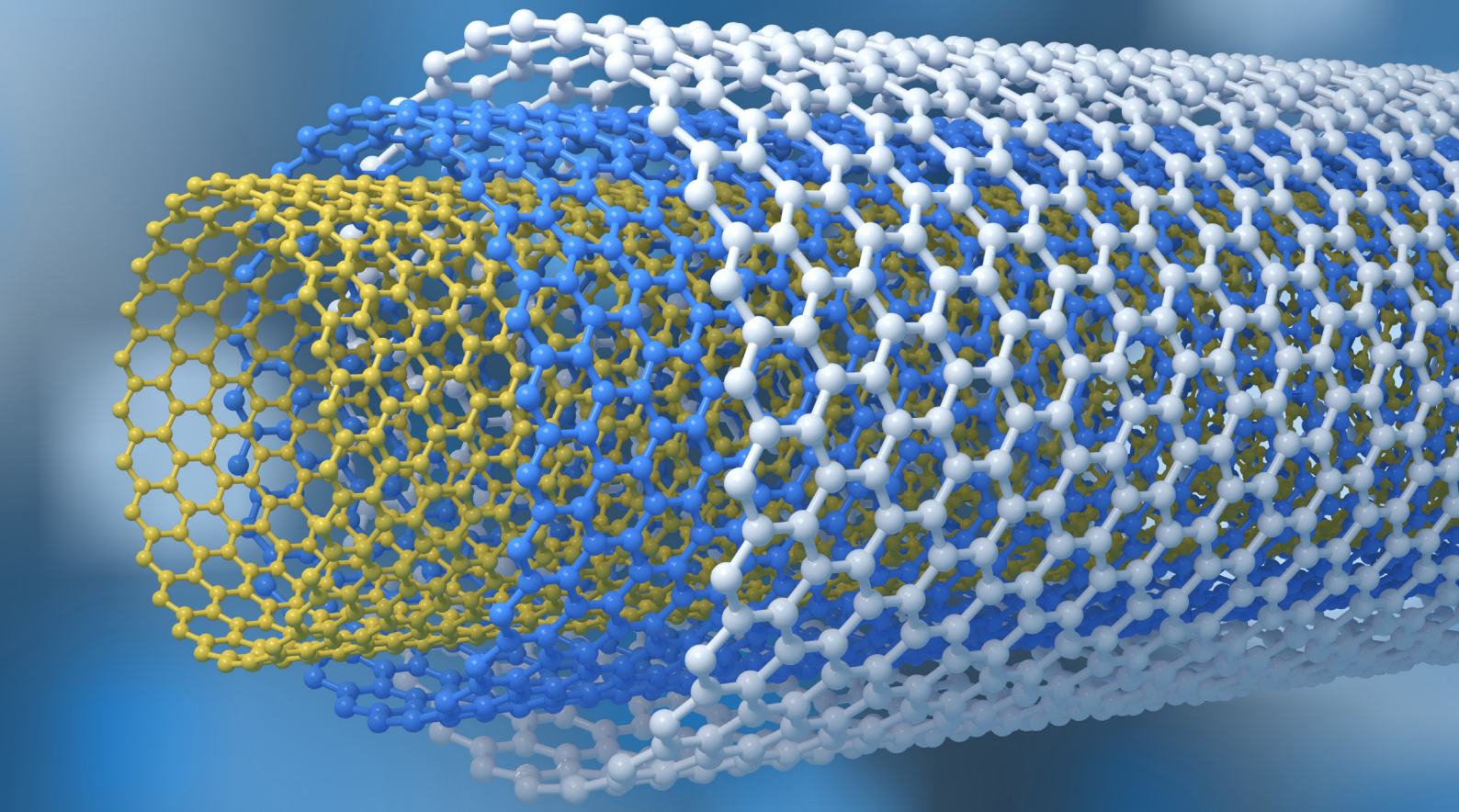

From stone to bronze and iron to the plastic and silicon of today — the materials we use and develop not only define periods of human history, but also determine our technological limits and possibilities. Researchers in chemical and materials sciences aim to expand these possibilities. In doing so, cutting-edge simulations performed on PRACE supercomputers help them to discover and design novel, exciting materials for our future. We present three projects pursuing different avenues to explore materials that are likely to raise our capabilities in electronics to a new level.

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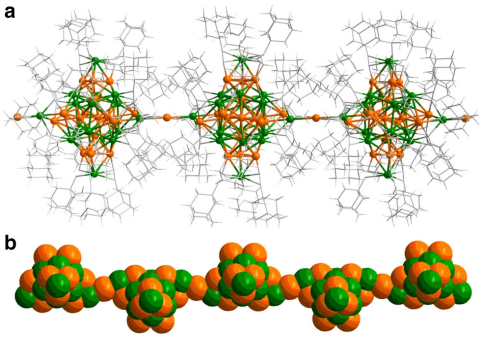
On the Nature of Self-assembly

Be it amino acids forming proteins or nucleotides assembling into DNA: Life happens by self-assembly. “Sometimes this is also the case in materials science,” says Hannu Häkkinen, a professor of computational nanoscience at the University of Jyväskylä, Finland. Together with colleagues from Xiamen University in China, his team investigated a unique type of gold-silver clusters consisting of 34 atoms, which can be induced to self-assemble into stable polymer chains simply by adding a certain organic solvent in the mixture.

“Such self-assembly reactions present an opportunity to use well-defined building blocks for designing nanomaterials with tuneable properties,” says Häkkinen. Using PRACE resources, he and his team modelled the novel nanomaterial’s structure and studied its electric properties. The results gave insights into the key role of the solvent in self-assembly. “The solvent molecules shield the reactive gold and silver atoms from the environment so that the clusters become building blocks that can be controlled,” explains Häkkinen. The calculations also confirmed a rather uncommon feature of the material: It is an electrical conductor in the direction along the fibres but an insulator in the other two directions. Going forward, computational methods could be used to vary cluster composition and solvent to explore other promising novel assemblies.

Supercomputing Resources:
MareNostrum 4 at BSC (Spain)



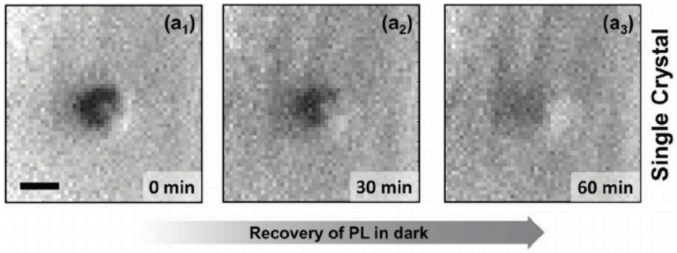
The self-assembled material is a linear polymer of 34-atom silver-gold clusters as building blocks. Gold atoms are orange, silver atoms are green, organic solvent molecules are grey. Image credit: Yuan et al. Nat. Commun. (2020).

How to Improve the Tolerance of Perovskites

Perovskites are peculiar materials: Because of a special characteristic of their electron orbitals, they are strongly tolerant towards material defects, which is the main reason why they are considered such promising materials for future electronic devices. “However, the defect tolerance is not consistent throughout the material”, says Simone Meloni, an Assistant Professor at the University of Ferrara. Apparently, the boundaries between crystalline grains in fabricated perovskites play a determining role in this. To better understand this phenomenon, Meloni and his co-workers performed molecular dynamics simulations using an archetypal perovskite (MAPbI3). They showed that defects, like the vacancy of an ion, indeed get trapped in energy minima occurring at grain boundaries.

The consequence of this behaviour became visible in lab experiments. While a sample consisting of one single crystal quickly recovered from a disruption by light-induced defects, the other sample, a poly-crystalline film containing many grain boundaries, hardly recovered at all. These insights point to the advantage of fabricating perovskite films with few crystalline grains — to safely avoid the grain boundary’s unfavourable effect.

Supercomputing Resources:
Piz Daint at CSCS (Switzerland), MARCONI (KNL) at CINECA (Italy)



A single crystal containing no grain boundaries quickly recovers after perturbation with light-induced defects. Image credit: Phung et al. Adv. Energy Mater. (2020).

Exploring the Landscape of 2D Materials

In recent years, 2D materials such as graphene have attracted great interest because of their exceptional optical and electrical properties. However, only a few dozen 2D materials have been experimentally investigated so far. Now, a team led by Nicola Marzari, professor of materials science at EPFL in Switzerland, has decisively increased the number of candidates to study. They have screened more than 100,000 inorganic compounds in high-throughput calculations, seeking to predict which ones could be obtained in a lab rather handily by exfoliation from the bulk 3D parent material. In a first run, the researchers identified roughly 1,000 easily exfoliable materials; now, in a second run using PRACE resources, they have doubled this count. “With this, the community suddenly has a wide portfolio of 2D materials to work with,” says Marzari.

The team also predicted the electronic properties of a number of these 2D materials and found several topological insulators, meaning materials that are insulators in their interior but possess conductive edges. Their tuneable electric resistivity could be used to generate a novel type of electronic components. Another star material that Marzari’s team investigated is the superconductor W2N3, for which they predicted a record high superconducting critical temperature of 22 Kelvin at ambient pressure — conditions which can be achieved using liquid hydrogen instead of the costly helium. “This is a very exciting find” says Marzari. He is convinced that, going forward, computational methods will further accelerate the identification of exciting 2D materials.

Supercomputing Resources: MARCONI (KNL) at CINECA (Italy).

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