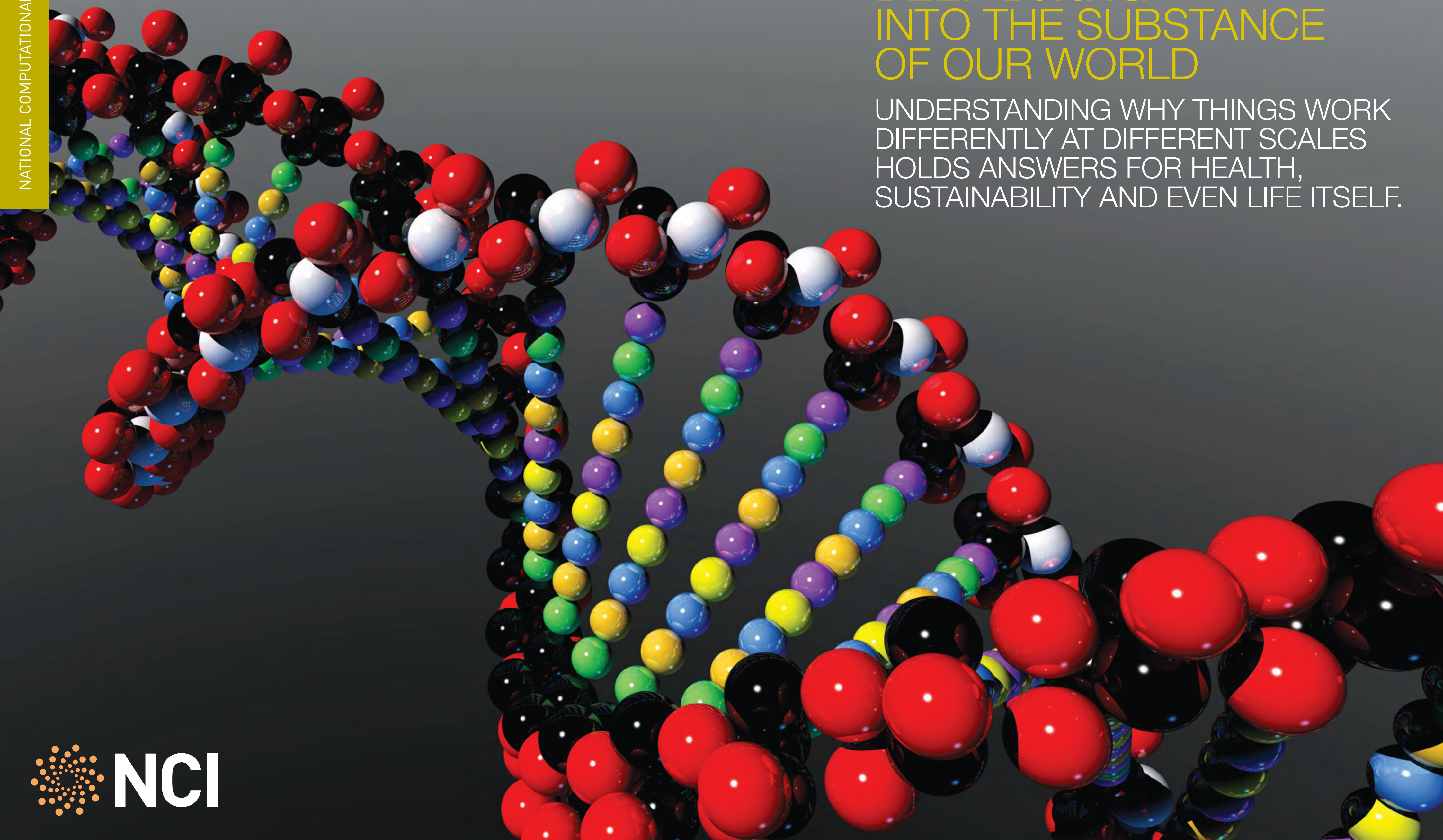
NATIONAL COMPUTATIONAL INFRASTRUCTURE

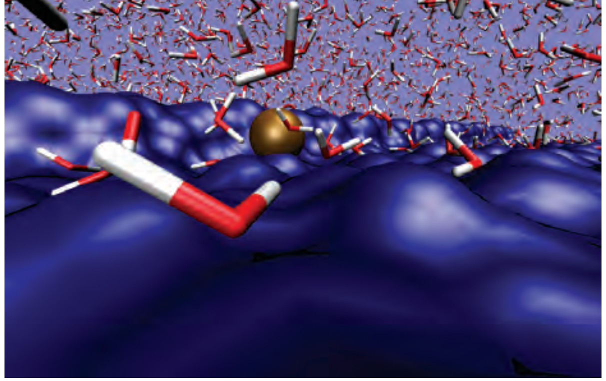
DEEP DIVING
INTO THE SUBSTANCE OF OUR WORLD

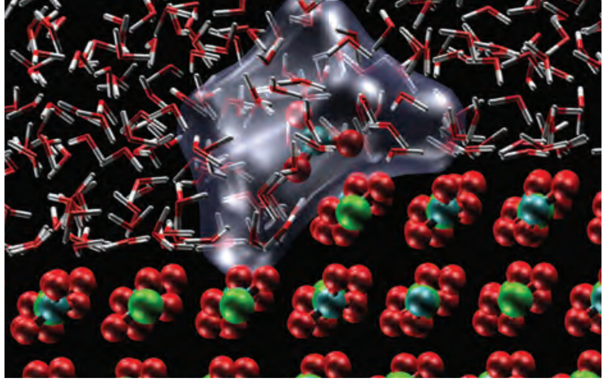
UNDERSTANDING WHY THINGS WORK DIFFERENTLY AT DIFFERENT SCALES HOLDS ANSWERS FOR HEALTH, SUSTAINABILITY AND EVEN LIFE ITSELF.



NCI

From exploring the earliest origins of life, to creating the quantum devices of the future, to unlocking a new source of fresh water for thirsty Australian cities, nanoscience involves discovering how the world works at the very smallest scales.





Professor Julian Gale of Curtin University and his team employ the vast computational power of the NCI supercomputer to see what goes on as the molecules that make up the stuff of our world assemble themselves in a multitude of ways to create different substances with often widely differing behaviours.

“It involves understanding how, at the molecular level, very small changes in the length or shape of objects can yield dramatically different electronic, mechanical or structural properties — in what is, essentially, the same material,” he says. “There are two huge challenges to exploring such systems: they are too tiny to manipulate experimentally with certainty — and yet they are too large and complex to calculate theoretically what is going on using conventional means. So we use atomistic computer simulation to model what happens both over time and at different scales.”

The research is pioneering new approaches that will be shared freely with Australian research organisations to help drive what many see as the coming revolution in advanced materials, devices and medicines, impelled by our growing ability to build things atom-by-atom or molecule-by-molecule to achieve particular, very precise purposes.

Many of Australia’s cities are becoming short of fresh water. Most States now plan to desalinate seawater to head off serious water shortages, but today’s filtration systems need vast amounts of energy to force water through the polymer membranes that remove the salt molecules. In so doing, they liberate large amounts of greenhouse gases, potentially adding to the very climate factors that cause rainfall to decline.

By probing what goes on in the membrane at the nano-level, Julian and his team are aiming to design a new generation of filters, equally or more efficient at removing salts, but requiring far less energy to push the water through and which are less inclined to block up.

Among the most tantalising assignments of the project is the quest for the origin of life itself. According to a current theory, the forefather molecules to the complex proteins and lipids of which all life consists formed in the boiling throats of hydrothermal vents on the seafloor. Here the complex interaction of sulphurous volcanic gases, heat, pressure and the catalysing effects of minerals containing iron, nickel and other metals formed substances ancestral to all living things. But the paths by which this might have occured are so vast in number the only way to find them is to explore the processes and see which lead to likely biological precursors. The team is carrying out extensive electronic structure calculations to probe the catalytic properties of the iron-sulphur-water interface to see how these early biomolecules might have arisen, with the added bonus that their work may reveal new ways to follow the example of these minerals by converting CO2 into useful but greenhouse-safe materials.

A third stream of the team’s work is exploring the formation, growth and shaping of materials to achieve different performances and outcomes. “Nature achieves all sorts of wonderful forms of the mineral calcium carbonate during biomineralisation to create bones, teeth, shells, the structures of diatoms or corals,” Julian says. “Unlocking the secrets of how to control molecular assembly to achieve such precise outcomes will have profound importance for the design of everything from pharmaceuticals to powerful new electronic devices and high performance materials.”

In a recent advance, the team explored a material that has the potential to increase the current available from lithium batteries by exploiting its more open nanoscale structure. Using computer models it was possible to explain why there can be a delay before the battery is able to release its energy.

Calculating the electronic properties of matter is a challenging problem, especially for nano-sized objects. Using standard approaches, it requires 8 times the computer power every time you double the number of atoms. Until recently this has restricted models to only a few hundred atoms at most. The program SIESTA, developed at Curtin in collaboration with Spanish scientists, greatly expands the horizons of such calculations by making the computational cost increase in proportion to the number of atoms. State-of-the-art computing facilities, such as NCI, are crucial to the goal of being able to explore the complex and fast-evolving world of nanoscience, Julian says.

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