NATIONAL COMPUTATIONAL INFRASTRUCTURE

FORESEEING THE UNFORSEEABLE— **WHEN THE LAWS OF NATURE CHANGE**

NANOTECHNOLOGY PROMISES A REVOLUTION IN NEW MATERIALS AND TECHNOLOGIES— BUT IT MUST ALSO BE SAFE, HEALTHY AND ENVIRONMENTALLY SOUND

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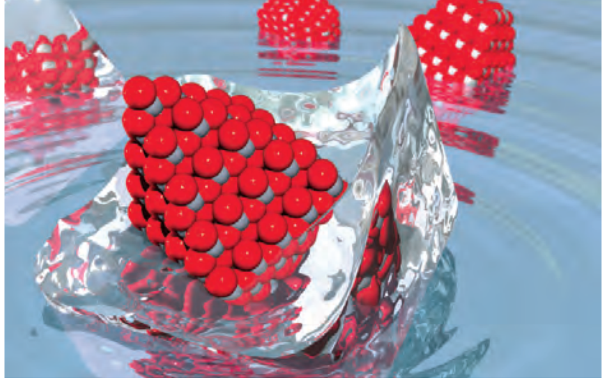
New materials never seen in Nature are starting to pour in their thousands from laboratories worldwide to build the electronic, medical and communication devices, the paints, plastics, catalysts and cosmetics of the future. With over 800 products already on the market globally, the nano-revolution is in full swing.



Above all Dr Amanda Barnard, of CSIRO's Virtual Nanoscience Laboratory, is concerned that this should be a safe revolution—that the new age should not be marred by the pollution, ill-health and hazards that resulted from past phases of 'dirtier' industrial development. Working at the international leading edge of the field, she is using the power of the NCI supercomputer to predict the properties of novel nanoparticles throughout their lives, searching for the flaws that might convert a benign substance into a dangerous contaminant.

"At this quantum mechanical scale the classical laws of physics don't apply," she explains. "Materials made from particles only billionths of a metre in size don't behave the same as larger objects. They are intrinsically unpredictable." Safe enough when made or used as intended in a consumer product, over their lifetimes the nanoparticles must nevertheless weather many changes in surrounding temperature, chemistry or pressure—and these may alter them in unforeseen ways.

Nanotechnology is being pursued so avidly precisely because, at this minute level, conventional substances take on unconventional attributes, which make them superior to the forms found in nature for transmitting electrons or photons, catalysing chemical reactions, or forming materials with rare and exceptional strength, flexibility or performance. Nanoparticles are synthesised by researchers in the lab mainly by using physical parameters such as temperature, pressure and pH to alter their structure and surface properties, the way their atoms align. They may be coated or treated in different ways. They are almost always stored or used under controlled conditions. Once released into the environment, however, they will be exposed to chemical and physical forces that may alter their fundamental properties in profound ways.

"We have to face the fact that, sooner or later, these substances will end up in garbage tips, flushed down the drain or free in water, soil or ecosystems, where they are exposed to all kinds of changes. We need to be certain that such changes will harm neither us nor the environment," Amanda explains.

Her research involves modelling how the surface chemistry and structure of these nanoscale objects can change when exposed to new conditions. It involves combining all configurations of the particle with all the many conditions it may encounter in the lab, in use or in the outside world, to predict whether it will remain stable—or shift to a different, potentially risky state.

"Laboratories round the world are churning out such a wide variety of engineered nanoparticles at such a rapid pace, that the task of systematically measuring the stability of all possible compositions, sizes and shapes in countless different chemical environments has already become impractically large," she explains. Her approach side-steps this problem by modelling all possible combinations and predicting where possible hazards may arise: these can then be tested experimentally in the laboratory. To achieve this Amanda has developed a new analytical multi-scale method—a general thermodynamic model which can be applied to any isolated nanostructure using parameters such as size, shape, temperature and chemical environment. It is, in effect, a standard safety screening method for any new nano-substance.

Even then, the computational task is vast. A single calculation for a single substance absorbs upward of 128 gigabytes of computer memory for anything up to 200 hours—and each substance requires dozens of runs. Only the NCI supercomputer can handle such tasks in a reasonable time, she says.

Her initial goal is establishing whether engineered nanoparticles formed from metals such as gold, platinum, palladium, nickel or copper are stable in air and water. From there the study will extend to embrace many different substances and conditions, including biological. Its overall aim is to develop a world-best system for testing almost any nano-substance under virtually any set of conditions. And from there, it will progress to calculations more complex still—from full environmental risk assessment to predicting consumer choices and social benefits flowing from nanoproducts.

While the chief focus of the research is on the need to protect society and the environment, it also offers major benefits to nanoscience itself. By investigating all the possible conditions a nanoparticle may encounter it will help to define its ideal operating conditions—and maybe even discover new and unexpected attributes and uses for it. This combination will help to place Australian nanoscience at the global forefront, for novelty, performance and—above all—for safety in the coming industrial age.

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