The virtual laboratory

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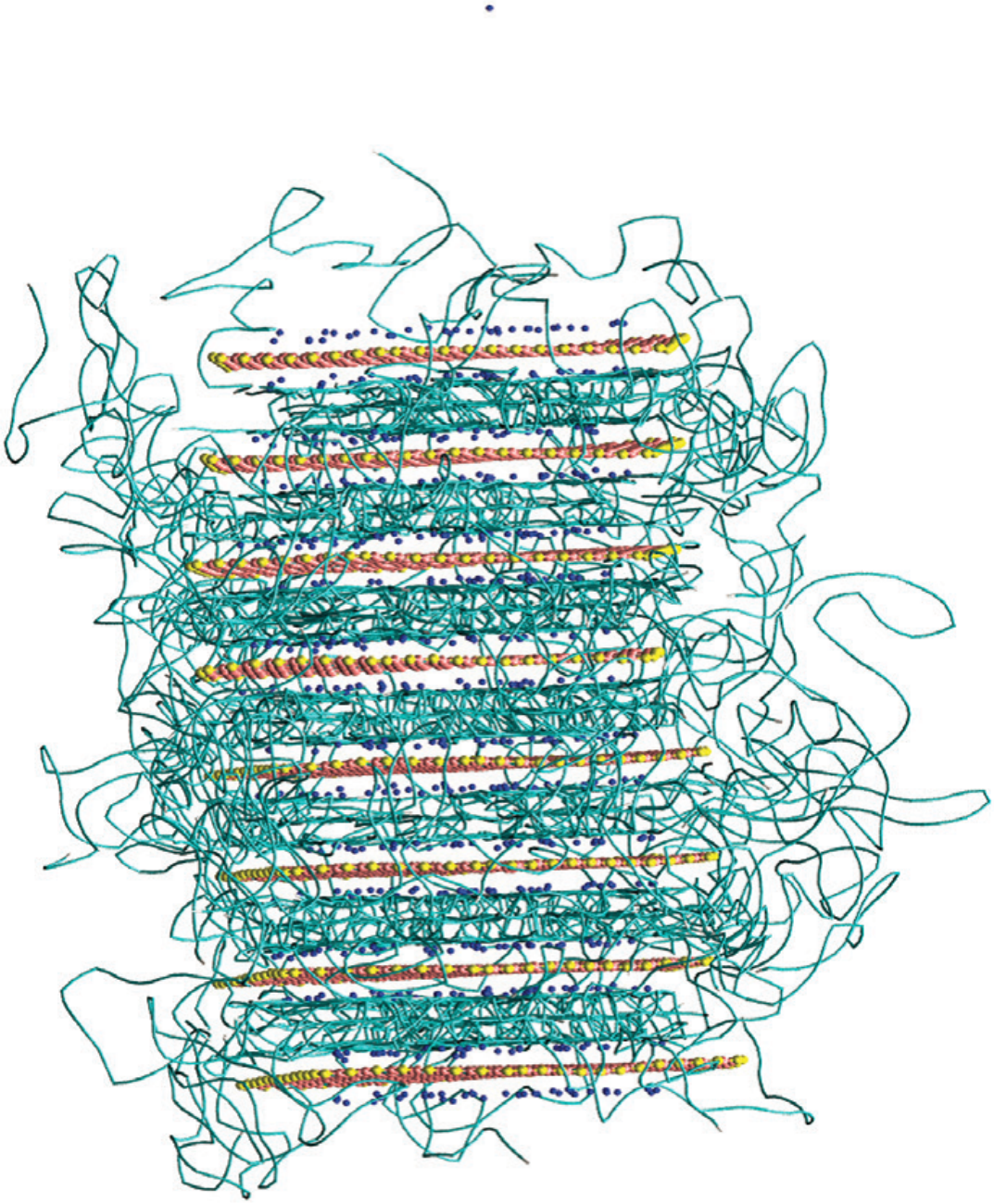

Figure 1: A snapshot from simulation of a self-assembled stack of clay layer and polymer molecules

Supercomputers can be used to simulate materials at vastly diverse scales, from the flow of air past an aeroplane's wing down to the movement of electrons around individual atoms. Different length and time scale domains provide different levels of information, but little is currently known about how these levels of information are connected. Professor Peter Coveney of University College London has been spearheading a long-term programme that aims to connect the scales, relating the behaviour of atoms and molecules to tangible properties at the macroscale.

In the late 1980s, researchers from Toyota demonstrated that by reinforcing polymers such as nylon with clay at the nanoscale, a significant improvement in a wide range of engineering properties could be made. Known as clay-polymer nanocomposites, these materials have very low density but are also tough and strong - ideal properties for the building of vehicles.

Extensive research into these materials has been going on ever since, and although there has been some success in finding useful new composites, it has proven to be difficult. The same researchers who made the initial discovery when working for Toyota recently wrote about the relative scarcity of such discoveries since their breakthrough almost thirty years ago, citing the laborious trial and error nature of the exploratory experiments required, but also a fundamental lack of understanding of how and why materials such as clay-polymer nanocomposites possess such anomalous properties.

Professor Peter Coveney of University College London, in collaboration with his colleagues Dr James Suter and Dr Derek Groen, has been working on ways of connecting different representations of matter together, which he believes is the first step towards speeding up the process of discovering new and useful materials. "Imagine, for example, a material that has fractured. At the molecular level, this is shown as the breaking of chemical bonds by electrons moving between atoms, whereas the manifestation on a larger scale would be the breaking of a component made of that material. These are very different representations of the same event, but both are equally correct. To simulate this event separately at different scales is relatively easy. What is not so easy is to connect the two - to extrapolate the macroscale properties of a material from its chemical composition."

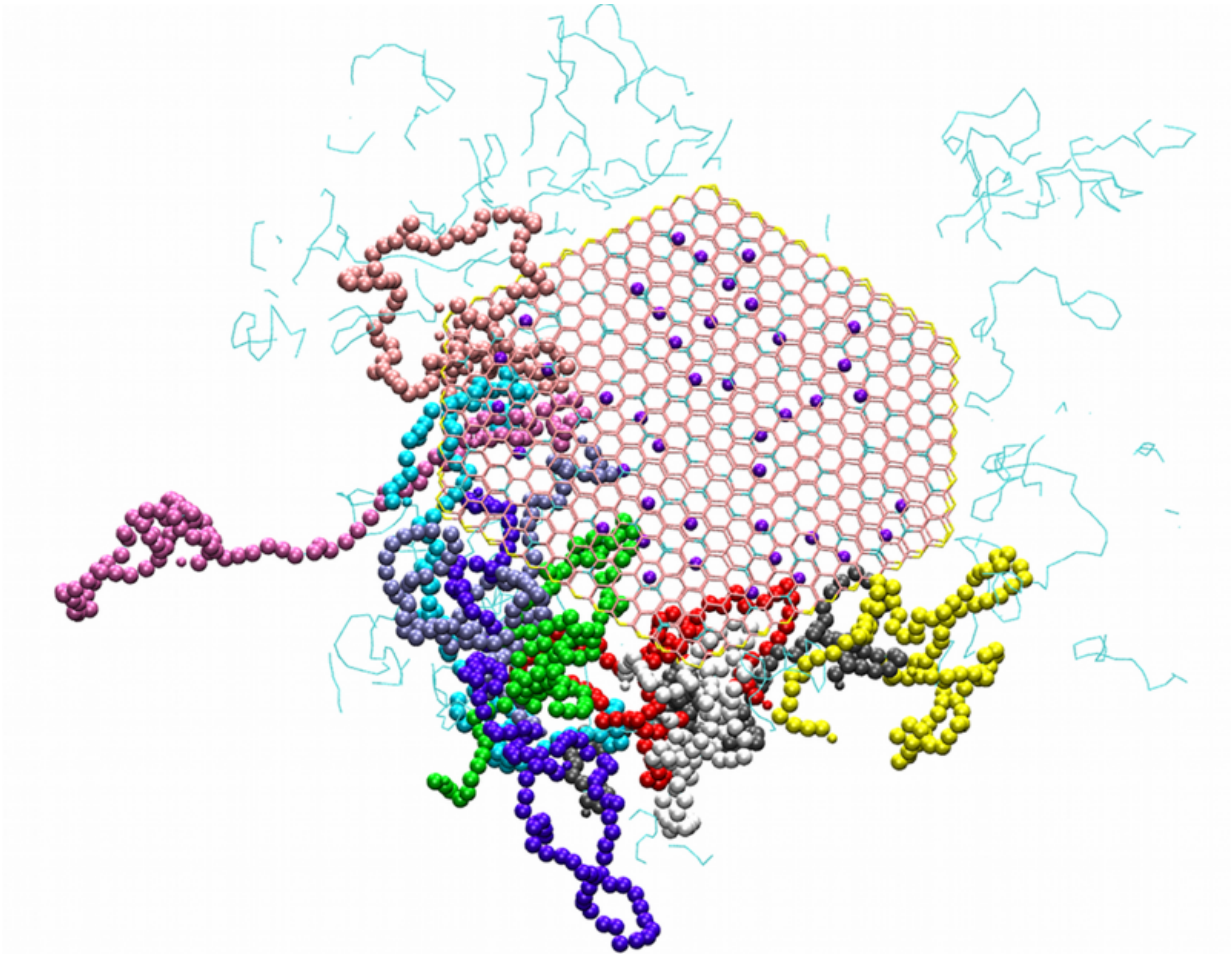

Figure 2: Illustration of the dynamic process of polymer intercalation between the hexagonal clay layers. Each polymer molecule is a different colour and moves rapidly through the interlayer spacing

Creating a description of a material that works at all scales without having to inject ad hoc parameters at higher levels is a crucial step towards in silico materials discovery. To pull off "multiscale modelling", as it is known, the lowest level parameters must be extremely precise, and the most powerful computers are needed in order to run the simulations. But the rewards for succeeding in this task are great; if one can predict the useful physical properties of a material from its molecular structure, then costly and time-consuming trial and error experiments can be eliminated from the discovery process.

In February 2015, the journal Advanced Materials published a paper by Suter, Groen and Coveney that discusses the properties of a number of claypolymer nanocomposites. However, it is not the specific materials that make the paper so interesting, but rather the groundbreaking methods behind the research. In the paper, they describe a method that can be used to calculate the properties of claypolymer nanocomposites using multiscale modelling. The only inputs needed for this "virtual laboratory" are chemical composition, molecular structure, and processing conditions, and in return it provides information that has largely never been shown before in any kind of modelling, let alone in an experiment.

"By connecting all the scales together into a multiscale model, we were able to show the process of polymers getting inside the clay layers - how it happens and how long it takes," says Coveney. "Clay exists naturally as

stacked sheets called tactoids. When you add a polymer, it will break up this natural configuration - encapsulating, exfoliating or intercalating the stacks. Our simulation showed that the composite then arranges itself in a particular orientation, such that the material properties begin to look very different from what you might predict from a linear combination of the properties of clay and the polymer."

The paper was considered so important by Advanced Materials that for the first time in its entire history the high impact journal published an extended feature so that the methods behind the work could be fully explained. "The ability to model and simulate the properties of a material in this manner has opened the door for making predictions that could vastly speed up many scientific discovery processes, not just in the field of clay-polymer nanocomposites," explains Coveney.

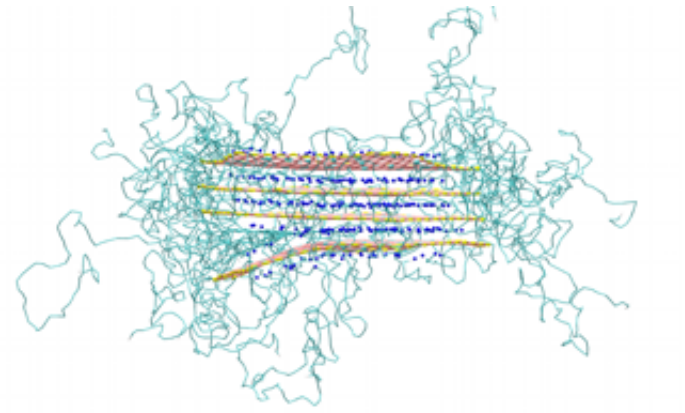

Figure 3: Coarse grained molecular dynamics simulation of poly(vinyl) alcohol polymer intercalating between layers of clay

Graphene, for example, is a material that has long been touted as a modern wonder material that will eventually revolutionise numerous fields of research. However, delivering the practical applications of

graphene has proven difficult, not least due to the challenges of producing it in large enough quantities. Multiscale modelling could be used to model the industrial production of graphene by exfoliating 2D sheets of graphene from graphite - a process fairly similar to the exfoliation of clay tactoids in the production of clay-polymer nanocomposites.

Coveney and his researchers have made extensive use of Tier-0 PRACE supercomputers, including 40.5 million core hours on JUGENE BlueGene/P at FZJ. "Carrying out multiscale simulations comes under the domain of what we call "heroic computing tasks", he says. "I personally believe that the future of materials science lies in gaining a proper understanding of composites, and this is very much dependent on the high fidelity nature of our models and simulations. Tier-0 supercomputers such as those provided by PRACE are absolutely essential for running these simulations in feasible time periods, and so the success of our work and any future work that uses our methods leans on the access that researchers have to these valuable resources."

In the short term, the team's methods have the potential to speed scientific discovery and understanding. In the long run, materials science will be changed for the better, by eliminating a lot of the trial and error that currently besets the development of useful materials.

More information: "Chemically specific multiscale modeling of clay-polymer nanocomposites reveals intercalation dynamics, tactoid self-assembly and emergent materials properties," *Advanced Materials*, 27 (6), 966-984 (2015), DOI: 10.1002/adma.201403361

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