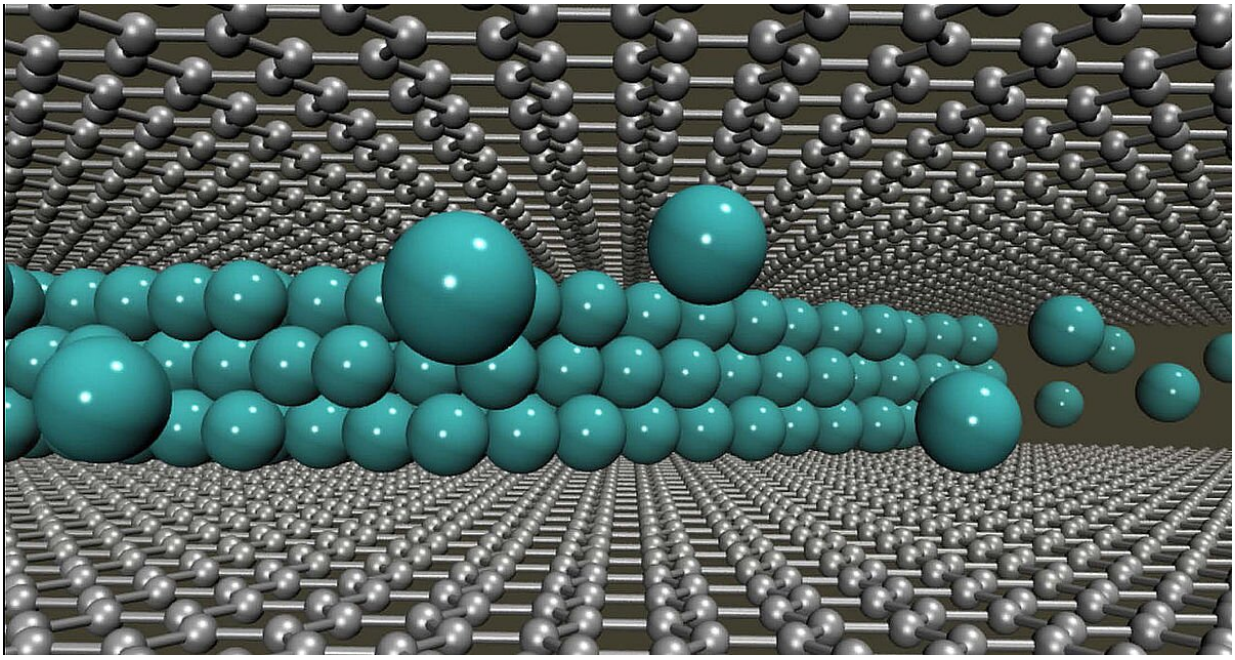
Supercomputing helps study two-dimensional materials

February 4 2019



Atomistic model illustrating a multilayer of lithium atoms between two graphene sheets. Credit: Dr. Mahdi Ghorbani-Asl, HZDR. See M. Kühne, et al., *Nature* 564 (2018).

Materials scientists study and understand the physics of interacting atoms in solids to find ways to improve materials we use in every aspect of daily life. The frontier of this research lies not in trial and error, though; to better understand and improve materials today, researchers must be able to study material properties at the atomic scale and under

extreme conditions. As a result, researchers have increasingly come to rely on simulations to complement or inform experiments into the properties and behaviours of materials.

A team of researchers led by Dr. Arkady Krasheninnikov, physicist at the Helmholtz-Zentrum Dresden-Rossendorf, collaborates with experimentalists to answer fundamental questions about material properties, and the team recently reported a breakthrough—the experimentalists were able to observe in real time the behaviour of lithium atoms when placed between two graphene sheets. A graphene sheet is a 2-D material, as it is only one atom thick, which made it possible to observe lithium atom motion in transmission electron microscopy (TEM) experiments.

With access to supercomputing resources at the Gauss Centre of Supercomputing (GCS), Krasheninnikov's team used the High-Performance Computing Center Stuttgart's (HLRS) Hazel Hen supercomputer to simulate, confirm and expand on the team's experimental findings. The collaborative work was recently published in *Nature*.

"Two-dimensional materials exhibit useful and exciting properties, and can be used for many applications, not only as a support in TEM," Krasheninnikov says. "Essentially, 2-D materials are at the cutting edge of materials research. There are likely about a couple thousand of these materials, and roughly 50 have actually been made."

Under the microscope

To better understand 2-D materials experimentally, researchers routinely use TEM. The method allows them to suspend small, thin pieces of a material and run a high-energy electron beam over it, ultimately creating a magnified image of the material that researchers can study, much like

a movie projector takes images from a reel and projects them onto a larger screen. With this view into a material, experimentalists can better chart and estimate atoms' positions and arrangements.

The high-energy beam can do more than just help researchers observe materials, though—it is also a tool to study the electronic properties of 2-D materials. Moreover, researchers can use the high-energy electrons from TEM to knock out individual atoms from a material with high precision to see how the material's behavior changes based on the structural change.

Recently, experimentalists from Max Planck Institute for Solid State Research, Stuttgart and the University of Ulm wanted to better understand how lithium particles interact between two atom-thin graphene sheets. Better understanding lithium intercalation, or placing lithium between layers of another material (in this case, graphene), helps researchers develop better battery technologies. Experimentalists obtained data from TEM and asked Krasheninnikov and his collaborators to rationalize the experiment using simulation.

Simulations allow researchers to see a material's atomic structure from a variety of different angles, and they can also speed up the trial-and-error approach to designing new materials purely through experiments. "Simulations cannot do the full job, but they can really limit the number of possible variants, and show the direction which way to go," Krasheninnikov says. "Simulations save money for people working in fundamental research and industry, and as a result, computer modelling is getting more and more popular."

In this case, Krasheninnikov and his collaborators found that the experimentalists' atomic coordinates, or the positions of particles in the material, would not be stable, meaning that the material would defy the laws of quantum mechanics. Using simulation data, Krasheninnikov and

his collaborators suggested a different atomic structure, and when the team re-ran its experiment, it found a perfect match with the simulation.

"Sometimes you don't really need high theory to understand the atomic structure based on experimental results, but other times it really is impossible to understand the structure without accurate computational approaches that go hand-in-hand with the experiment," Krasheninnikov says.

For the first time, the experimentalists watched in real time how lithium atoms behave when placed between two graphene sheets, and with the help of simulations, gained insights into how the atoms were arranged. It was previously assumed that in such an arrangement, the lithium would be structured as a single atomic layer, but the simulation showed that lithium could form bi- or trilayers, at least in bi-layer graphene, leading researchers to look for new ways to improve battery efficiency.

The team effectively ran first-principles simulations of 1,000-atom systems over periods of time to observe short-term (nanosecond time scale) material interactions. Larger core counts on next-generation supercomputers will allow researchers to include more atoms in their simulations, meaning that they can model more realistic and meaningful slices of a material in question.

The greater challenge, according to Krasheninnikov, relates to how long researchers can simulate material interactions. In order to study phenomena that happen over longer periods of time, such as how stress can form and propagate a crack in metal, for example, researchers need to be able to simulate minutes or even hours to see how the material changes. That said, researchers also need to take extremely small time steps in their simulations to accurately model the ultra-fast atomic interactions. Simply using more computer cores allows researchers to do calculations for larger systems faster, but cannot make each time step go

faster if a certain parallelization threshold is reached.

Breaking this logjam will require researchers to rework algorithms to calculate more efficiently each time step across a large number of cores. Krasheninnikov also indicated that designing codes based on quantum computing could enable simulations capable of observing material phenomena happening over longer periods of time—quantum computers may be perfect for simulating quantum phenomena. Regardless of what direction researchers take, Krasheninnikov noted that access to supercomputing resources through GCS and PRACE enables him and his team to make continual progress. "Our team cannot do good research without good computing resources," he said.

More information: Matthias Kühne et al, Reversible superdense ordering of lithium between two graphene sheets, *Nature* (2018). DOI: 10.1038/s41586-018-0754-2

Provided by Gauss Centre for Supercomputing

Citation: Supercomputing helps study two-dimensional materials (2019, February 4) retrieved 25 April 2024 from https://phys.org/news/2019-02-supercomputing-two-dimensional-materials.html

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