need for the photocopies. This was allowed because there was deemed to be sufficient national interest in the ruling.

Liang was involved in that case, and says that India's fair-dealing provisions could be broad enough to facilitate the kind of access that Sci-Hub gives to articles. As with the textbooks, national interest in the case means that affected parties can submit evidence to the court. Earlier this year, 20 of India's leading scientists argued that the country's scientific community "stands to be gravely prejudiced" if the case goes against Sci-Hub.

The scientists say in a document – known as a petition – submitted to the court that the case could have an "adverse impact on access to scientific knowledge, and so on science and technology research in India".

"Access to information is crucial for researchers. When the information is hidden behind paywalls, that curbs innovation," says Shahid Jameel, a virologist currently at the University of Oxford, UK, who signed the petition. Computational biologist Rahul Siddharthan at the Institute of Mathematical Sciences in Chennai, India, adds that "apart from a small number of elite institutes in India, most cannot afford to subscribe" to journals.

Further petitions supporting Sci-Hub have been submitted by medical doctors and policy advisers who use scientific papers as part of their work.

Ripple effect

The case's next hearing is scheduled for 16 December, but legal experts warn that it could rumble on for years. Scaria says that the outcome will depend on whose rights the judge focuses on under the copyright rules. "If the judge views the matter from the perspective of user rights under copyright law, there is a high chance that Sci-Hub will win the case," he says. But if the judge views the matter from the perspective of the copyright holder, the verdict might go against the site.

The ramifications for publishers if Sci-Hub wins are hard to predict, say Sci-Hub's lawyers Shrutanjaya Bhardwaj and Sriya Sridhar. "Courts in progressive nations frequently borrow principles from foreign jurisdictions, and it is possible that Sci-Hub's victory before the Delhi high court will cause a global ripple effect," they say. A loss for Sci-Hub could see many researchers and institutions that cannot afford journal subscriptions being "excluded from access to scholarly work", they add.

Elbakyan says that the case could change everything for Sci-Hub. Winning could bring opportunities to improve the site and extend its reach.

"Today, the perception of Sci-Hub [is that] it is an illegal project, and that is even not disputable, but a fact," she tells *Nature*. "Victory will show the 'fact' to be merely an opinion."

DEEPMIND AI TACKLES ONE OF CHEMISTRY'S TOP TECHNIQUES

Machine-learning algorithm predicts material properties using electron density.

By Davide Castelvecchi

A team led by scientists at the London-based artificial-intelligence company DeepMind has developed a machine-learning model that suggests a molecule's characteristics by predicting the distribution of electrons within it. The approach, described in the 10 December issue of *Science*, can calculate the properties of some molecules more accurately than existing techniques (J. Kirkpatrick *et al. Science* **374**, 1385–1389; 2021).

"To make it as accurate as they have done is a feat," says Anatole von Lilienfeld, a materials scientist at the University of Vienna.

The paper is "a solid piece of work", says Katarzyna Pernal, a computational chemist at Lodz University of Technology in Poland. But she adds that the machine-learning model has a long way to go before it can be useful for computational chemists.

Predicting properties

In principle, the structure of materials and molecules is entirely determined by quantum mechanics, and specifically by the Schrödinger equation, which governs the behaviour of electron wavefunctions. These

> **"It's sort of the ideal problem for machine learning: you know the answer, but not the formula you want to apply."**

are the mathematical gadgets that describe the probability of finding a particular electron at a particular position in space. But because all the electrons interact with one another, calculating molecular structures and orbitals from such first principles is a computational nightmare, and can be done only for the simplest molecules, such as benzene, says James Kirkpatrick, a physicist at DeepMind.

To get around this problem, researchers have for decades relied on a set of techniques called density functional theory (DFT) to predict molecules' physical properties. The theory does not attempt to model individual electrons, but instead aims to calculate the overall distribution of the electrons' negative

electric charge across the molecule. "DFT looks at the average charge density, so it doesn't know what individual electrons are," says Kirkpatrick. Most properties of matter can then be easily calculated from that density.

Since its beginnings in the 1960s, DFT has become one of the most widely used techniques in the physical sciences: an investigation by *Nature*'s news team in 2014 found that, of the top 100 most-cited papers, 12 were about DFT.

But the approach has limitations, and is known to give the wrong results for certain types of molecule. And although DFT calculations are vastly more efficient than those that start from basic quantum theory, they are still cumbersome and often require supercomputers. So, in the past decade, theoretical chemists have increasingly started to experiment with machine learning, in particular to study properties such as materials' chemical reactivity or their ability to conduct heat.

The DeepMind team has made probably the most ambitious attempt yet to use AI to calculate electron density, the end result of DFT calculations. "It's sort of the ideal problem for machine learning: you know the answer, but not the formula you want to apply," says Aron Cohen, a theoretical chemist at DeepMind.

The team trained an artificial neural network on data from 1,161 accurate solutions derived from the Schrödinger equations. To improve accuracy, they also hard-wired some of the known laws of physics into the network. They then tested the trained system on a set of molecules that are often used as a benchmark for DFT, and the results were impressive, says von Lilienfeld. "This is the best the community has managed to come up with, and they beat it by a margin," he says.

One advantage of machine learning, von Lilienfeld adds, is that although it takes a massive amount of computing power to train the models, that process needs to be done only once. Individual predictions can then be done on a regular laptop, vastly reducing their cost and carbon footprint.

Kirkpatrick and Cohen say that DeepMind is releasing their trained system for anyone to use. For now, the model applies mostly to molecules and not to the crystal structures of materials, but future versions could work for materials, too, the authors say.