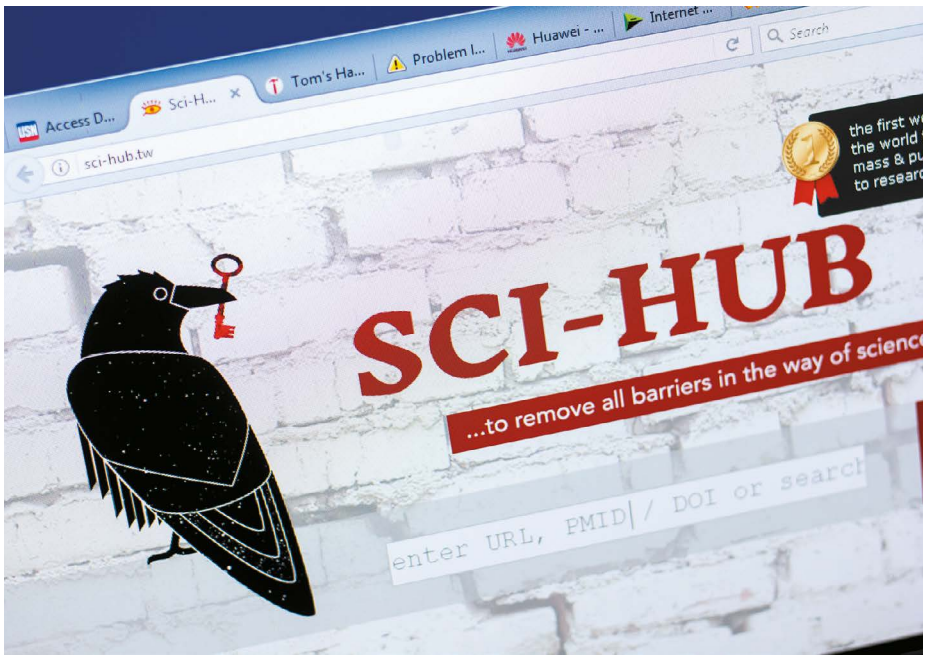

Sci-Hub argues that its activities are permitted under India's copyright law.

SHARAF MAKSUMOV/SHUTTERSTOCK

WHAT SCI-HUB'S LATEST COURT BATTLE MEANS FOR RESEARCH

Delhi court will scrutinize whether the pirate paper website falls foul of India's copyright law.

By Holly Else

Sci-Hub, the popular website that offers access to millions of pirated research papers and books, is no stranger to legal action. But, for the first time, the site is defending its operations in court, in a copyright case filed in India by a group of major publishers.

In a lawsuit presented in Delhi's high court, the American Chemical Society, Elsevier and Wiley say that the site infringes their copyright, and ask the court to instruct Internet service providers in India to block access to it.

Sci-Hub's founder Alexandra Elbakyan argues that, in India, copyright is "not applicable in cases such as Sci-Hub, when [material] is required for science and education".

Legal experts say that there is a chance the court will rule in Sci-Hub's favour, because of a key aspect of the country's copyright law. The case hinges on the definition of 'fair dealings', which in the past has enabled institutions in India to lawfully reproduce academic textbooks and other copyrighted material for use in education.

If Sci-Hub wins, it could force publishers to rethink their business models in a similar way to how the music industry changed in response to the arrival of the Internet, says Arul George Scaria, a legal scholar at the National Law University, Delhi. Attitudes towards Sci-Hub in other countries could change on the basis of India's ruling, and the outcome could even influence similar cases in future.

Pirate site

Previously, publishers have sued Sci-Hub and Elbakyan in several countries, and access has been blocked, or is due to be blocked, in 11 countries, including Germany, France, Sweden and the United Kingdom.

"There are serious questions of access to knowledge that the court ought to take into account."

In lawsuits filed in recent years by Elsevier and the American Chemical Society, US judges ruled that Sci-Hub infringed the publishers' copyrights and owed them US$15 million and $4.8 million, respectively. Elbakyan did not appear in court, or offer any legal representation for the site during those cases, and the fines have so far not been paid.

"Pirate sites like Sci-Hub threaten the integrity of the scientific record, and the safety of university and personal data," the publishers behind the case in India told Nature in a statement. "They compromise the security of libraries and higher-education institutions, to gain unauthorized access to scientific databases and other proprietary intellectual property, and illegally harvest journal articles and e-books." The publishers also allege that Sci-Hub uses stolen user credentials and phishing attacks to extract copyrighted journal articles illegally.

Elbakyan says that these are "empty accusations" that "have absolutely no content of evidence behind them". She denies that Sci-Hub is a threat to science, or to the security of academic institutions. "Open communication is a fundamental property of science and it makes scientific progress possible. Paywalled access prevents this," Elbakyan adds. "That is a threat, and not Sci-Hub."

The site has proved popular among researchers, who say their institutions cannot afford costly journal subscriptions. India accounts for the third-largest proportion of Sci-Hub's users, and when publishers brought the Delhi case in December 2020, a group of lawyers offered Elbakyan legal representation.

"There are serious questions of access to knowledge that the court ought to take into account," says Lawrence Liang, a legal scholar at Ambedkar University Delhi, who isn't part of the defence team but helped to rally support for Sci-Hub from scientists.

Fair dealings?

The defence will argue that Sci-Hub's activities are covered by the list of exemptions in India's Copyright Act of 1957. One of these is that 'fair dealings' of a work can be used for private or personal use, including research.

Academic publishers have fallen foul of this section of the act before. In 2012, five publishers — including Oxford University Press and Cambridge University Press — unsuccessfully sued the University of Delhi and its photocopying shop for alleged copyright infringement in course packs made at the institution. These packs contained photocopies of passages and chapters from textbooks and, in some cases, copies of entire books that were produced for students, many of whom could not afford to buy the originals.

The judge ruled that the university and the photocopying shop were not infringing the copyright of the books' publishers, because one of the exemptions listed in the copyright act includes reproducing work "by a teacher or pupil in the course of instruction". A key part of the case was evidence submitted to the court by students and teachers stating the

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 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.

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

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.