FEATURE ARTICLE

Leveraging Spintronics

A Computer Code that can Hunt for Ferromagnetic Materials

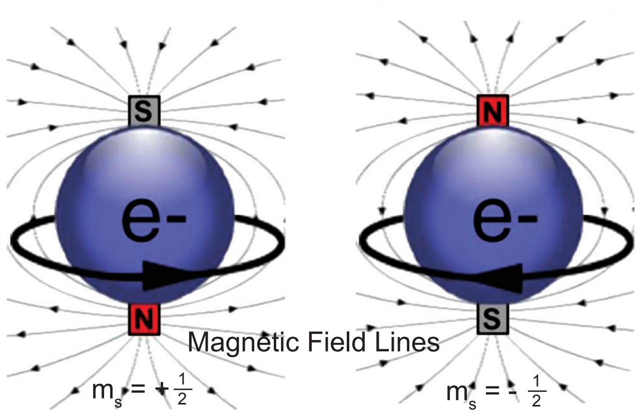
Susheela Srinivas

IN recent years, researchers are increasingly exploring two-dimensional (2D) electronic-grade materials to exploit them in semiconductor devices. Made up of single-layer, atom-thick crystal structures, 2D materials exhibit unique properties. They no longer follow the natural laws of physics seen in bulk materials, instead, are governed by quantum laws. They display a broad range of useful electrical, mechanical and optical properties with tremendous potential to revolutionise next-generation electronic devices: by offering nano-scale integration, ultra-high-speed of operation and low power consumptions.

For decades, it was believed that 2D materials do not exhibit ferromagnetism. However, in 2017, scientists discovered that two 2D materials — Chromium Iodide and CGT ($Cr_2Ge_2Te_6$) — are inherently ferromagnetic. Their study opened new possibilities to explore a variety of magnetic materials such as ferromagnetic, half-magnetic, and paramagnetic. All of them with potential use as electronic grade materials. Since then, several 2D materials have been theorised and classified under this category.

Spintronics

Electrons are charge-carrying elements that move around the nucleus. They also possess a spin and an angular momentum. The combination of these two – electrical charge and spin momentum – gives rise to small magnetic energy, which is similar to the magnetic field generated by a current-carrying conductor. The spin has two states – up and down – giving rise to a polarity of the magnetic field, which is also a measurable quantity.



The magnetic field of electron spin (*Courtesy: scind.org*)

"Many materials exhibit this inherent magnetic property at the atomic level," says Dr Santanu Mahapatra, Professor, Nano-Scale Device Laboratory at the Indian Institute of Science (IISc), Bengaluru. "However, only when a substantial number of electrons have their spins aligned in one direction, they add up to generate a unidirectional magnetic property in the material," he explains. An example of aligned spins is a ferromagnetic material that exhibits magnetism. Whereas if the individual electron spins are in opposing directions, the overall magnetic field is neutralised.

Present-day devices control the electron charge current through semiconducting materials and utilise it to perform various tasks. Information is encoded in several million devices embedded in modern-day electronic chips or ICs. The devices process the data in terms of logic 1 (presence of charge) and logic 0 (absence of charge).

However, in the past few years, scientists are looking to exploit the small magnetic fields generated by the electron spins instead of using their charge as information carriers. By encoding the information in the spin state (up-spin is logic 1, and down-spin is logic 0), the ICs can operate at much higher efficiencies.

This emerging technology is called Spintronics (spin-electronics) which relies on manipulating the spin direction of the electrons and use it for information storage.

Researchers project several advantages of this technology. Firstly, very little electrical energy is required to change the spin direction, thereby drastically reducing power consumption in the chips. So instead of using electrical power to drive a charge current through a semiconductor device, Spintronics uses a fraction of the input power to change the spin direction of the electrons of the material. Second, spin states can be set very quickly, facilitating the rapid rate of information transmission. And third, such information is non-volatile, implying, once the spin states are set, they remain in these states without the need for external power backup for data storage.

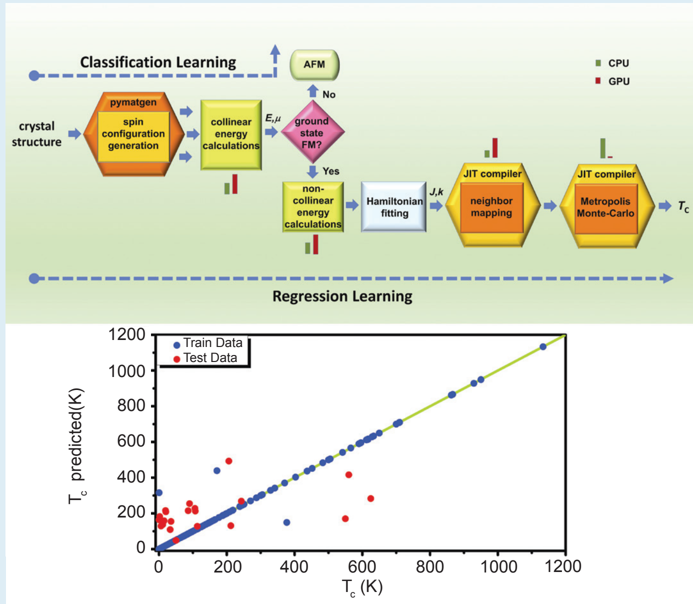
New-age Materials

Evidently, magnetic materials assume importance for fabricating spintronic devices. In recent years, the design of devices such as magnetic tunnelling junction transistors, have spurred the investigation of various other materials that could be useful for spintronics. In this endeavour, exotic properties of 2D materials like half metallicity and half-semiconducting nature have further added impetus to new age electronic grade

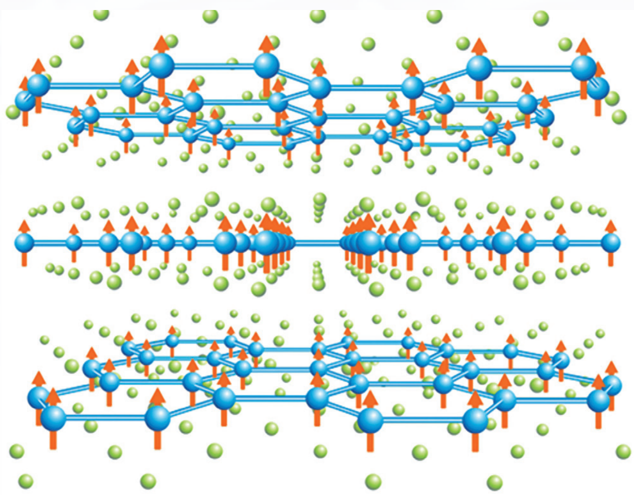
How the Machine Learns

"The dataset in our work is like a matrix with each row represented by material, and each column represents a specific feature of the material," explains Arnab Kabiraj, first author of the study. Their dataset contained 157 materials, each with 1500 properties. "We then employed a 3-part method of processing," he elaborates:

1. Select Percentile – the dataset columns are reduced by selecting the best features and discarding the irrelevant ones.
2. Zero Counts – all zero-valued data generated after step 1 are eliminated at this stage.And finally, the data is subjected to a standard supervised Machine Learning technique.
3. Gradient Boosting Regressor – an ensemble-based model that uses a predictor – like a decision tree – to enhance performance.



The different building blocks of the software (above); Accuracy of machine learning model compared with the software predicted value (Kabiraj *et al.*)



Ferromagnetism in 2D materials (Courtesy: physicstoday.org)

materials. By using such advanced materials, there is an exciting possibility of building innovative spintronic devices and circuits. Also, 2D materials offer an additional attraction of having atomically thin structures, making ultra-small devices and ultra-high integration possible.

When in 2017, scientists discovered combination ferromagnetic 2D materials, it opened floodgates to investigate several other blends of materials that have potential use in spintronics.

The Curie Point

The magnetic property of 2D ferromagnets (2DFM) begins to decline with rising temperatures. At one critical temperature called the Curie point, the material loses its ferromagnetism. Curie point of 2DFM is, therefore, a crucial aspect of consideration for practical applications. Most of the experimentally synthesised 2D materials show low-temperature magnetism, whereas 2D-based devices require ferromagnetism at higher operating temperatures. The quest for such elements has intensified over the past few years.

The Hurdles

Selecting a suitable 2D material and calculating its Curie point is a complicated process involving the integration of the crystal structure, analysis, and individual spin-configurations. After which, intensive, complex computations have to be performed to determine the Curie points of 2D materials suitable for Spintronics. Presently, the procedure is a heuristic-based, manually intensive process. Gleaning information from an extensive database comprising thousands of entries, and performing calculations on them is fraught with many challenges.

Simplifying the Process

Now, Indian researchers have simplified the process with a computer-based solution. The research team from the IISc

The research team from IISc

comprising, Arnab Kabiraj, Mayank Kumar and Santanu Mahapatra, have developed an open-source, fully-automated computer code that can estimate the Curie temperatures of 2D materials from their crystal structures. Their study, published this April in Nature - *npj Computational Materials,* utilises open source databases and combines informatics and machine learning to automatically predict the material's Curie temperature. The main objective of this work is to find 2DFM materials with high Curie point from the materials database, thereby minimising human errors.

"In the conventional procedure, there is a high probability of missing out some spin configurations. These oversights are eliminated by our automated process," says Dr Mahapatra, principal investigator of the study.

The Robust Coding

The team chose a database of nearly 800 known 2D materials and applied their crystal structures as input for the algorithm. The team employed cutting-edge processor technology, combining both graphical and central processing units. Along with this, advanced computer programs like just-in-time compilers performed the large scale complex computations on the structural data. The program can simultaneously calculate Curie points of four materials without human intervention within 10 hours even in a workstation with GPU acceleration.

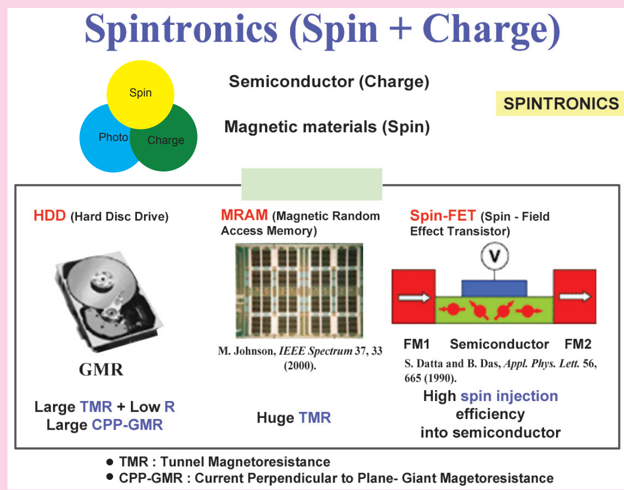
Their study also revealed that nearly 47% of the source database (of the 800 materials) were erroneously categorised as ferromagnetic. Also, the program sourced out high-temperature 2DFM potential spintronic materials: 26 materials that work at 400K (around 127 degree Celsius) and about 32 materials that can operate at 300K (approximately 27-degree Celsius).

Besides, their study highlighted magnetic properties in uncategorised materials — those containing Molybdenum, Tungsten and Titanium.

A Sea Change in Storage Capacity

The 2007 Nobel prize in Physics was awarded jointly to Albert Fert and Peter Grünberg for the discovery of Giant Magnetoresistance (GMR). GMR is the sudden change in electrical resistance in alternating layers of ferromagnetic and non-magnetic metal layers when exposed to a magnetic field. The resistance change occurs due to scattering of electron spins in the different layers.

By using GMR technology, individual data bits can be stored in smaller areas on devices such as magnetic hard-disk drives and in designing small and sensitive read heads – a standard feature in nearly all computers of the present day.



Concepts and applications of spintronics
(©K. Inomata, Via Research Centre for Magnetic and Spintronic Materials)

A Step Ahead

The team further scaled their work by applying a Machine Learning algorithm to their program. "Presently we have selected 157 data points incorporating general chemical features of the materials, from which the output automatically predicts the Curie Temperature," says Dr Mahapatra. Although this is a small input dataset, it provides an initial platform for an Artificial Intelligence-based system of assessing 2D-FM materials for use in Spintronics.

The work also sets an example of how computational techniques can be used to get insights into emerging nanoscience. It provides a means to detect broad range 2DFM materials quickly and accurately from which experimentalists can perform further rigorous analysis for specific applications.

"India lacks indigenous scientific software, our study will encourage young researchers to develop cutting-edge scientific codes," opines Dr Mahapatra.

Ms Susheela Srinivas is a Bengaluru-based science communicator.