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A sustainable spin to energy-efficient computers and smart phones.

The journey to net zero carbon is complex but essential, and as such is encouraging scientists to approach research from different angles, combining techniques and tools in original ways to explore new materials for improved greener solutions.

Dr Ivan Scivetti and Dr Gilberto Teobaldi - both based at the Science and Technology Facilities Council (STFC) Scientific Computing Department - have done exactly that. Their work is exploring a new sustainable option in the science of spintronics, a commercial technology for magnetic information storage and processing, and used in electronic products such as computers, smart TVs and mobile phones.

The Issue

The field of spintronics is relatively new and, so far, based on compounds comprising metals that are rare and expensive to extract from the earth, and to purify. This involves harsh and hazardous chemical processes that add additional manufacturing challenges and costs to spintronic technologies. In addition, the geopolitical issues in terms of their mining, resourcing and distribution all combine to form a strong motivation to find alternatives that are based on cheaper and more environmentally benign elements.

In a simplified picture, electrons exist in one of two spin states: ‘up’ or ‘down’. Electrons of opposite spin states can have distinct electron-transport properties - i.e. electrical conductivity. If the electrons in one spin state conduct electricity whereas the electrons in the other spin state do not, the material is half-metallic. Half-metals are capable of selectively transporting electrons of only one spin-state. This is a highly sought after property for spintronics applications that require the flowing of electron-spins - or spin-currents.

“Without these rare-earth metals, spintronic devices can’t function properly. Our research, which uses advanced computer simulations to test research data and ideas, has revealed a promising alternative that is both cheaper and more abundant than the rare-earth metals currently used in computers, smart TVs and mobile phones.”

-Dr Ivan Scivetti

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Spin-currents do not dissipate energy as heat, resulting in devices of substantially increased energy efficiency in comparison to standard commercial solutions based on electron-currents - i.e. the flowing of electricity. Unfortunately, while relatively common in materials containing rare-earth metals, such properties are not typically present in compounds of cheap and benign transition-metals such as manganese (Mn).

Our Approach

Drs Scivetti and Teobaldi approached this challenge from a different perspective, applying research strategies from surface science and computational physics to a metal oxide material (lithium-manganese-oxide, $LiMn_2O_4$) typically used for battery applications. They used quantum mechanical simulations to model thin films of $LiMn_2O_4$ under geometric strain - stretch and compression - and investigate how these factors influence the film's electronic and magnetic properties.

The two researchers modelled different crystallographic planes of $LiMn_2O_4$ and simulated them under varying amounts of strain. They found that, when placed under strain, the interplay between strain and different chemical compositions (the specific amount of lithium, manganese and oxygen in each plane of the layered material) determine the system's metallic and magnetic properties, and consequently their spin - and electron - conductivity.

This computational screening pointed out several unexpected half-metallic solutions for different compositions of strained $LiMn_2O_4$ films.

Benefits

The observed half-metallic properties and predicted response to strain endows $LiMn_2O_4$ films with the capability of spin-selective electron transport in the absence of any rare-earth metal in the system, indicating more sustainable avenues to sourcing materials for spintronics applications.

"This work provides unexpected insights that will inform new research avenues for the development of more sustainable, energy-efficient electronic devices than commercially used, or being considered for use, throughout the world today."

-Dr Gilberto Teobaldi

Further information

The paper 'Combined Role of Biaxial Strain and Nonstoichiometry for the Electronic, Magnetic, and Redox Properties of Lithiated Metal-Oxide Films: The $LiMn_2O_4$ Case', is published in ACS Applied Materials and Interfaces https://pubs.acs.org/doi/10.1021/acsami.1c18326

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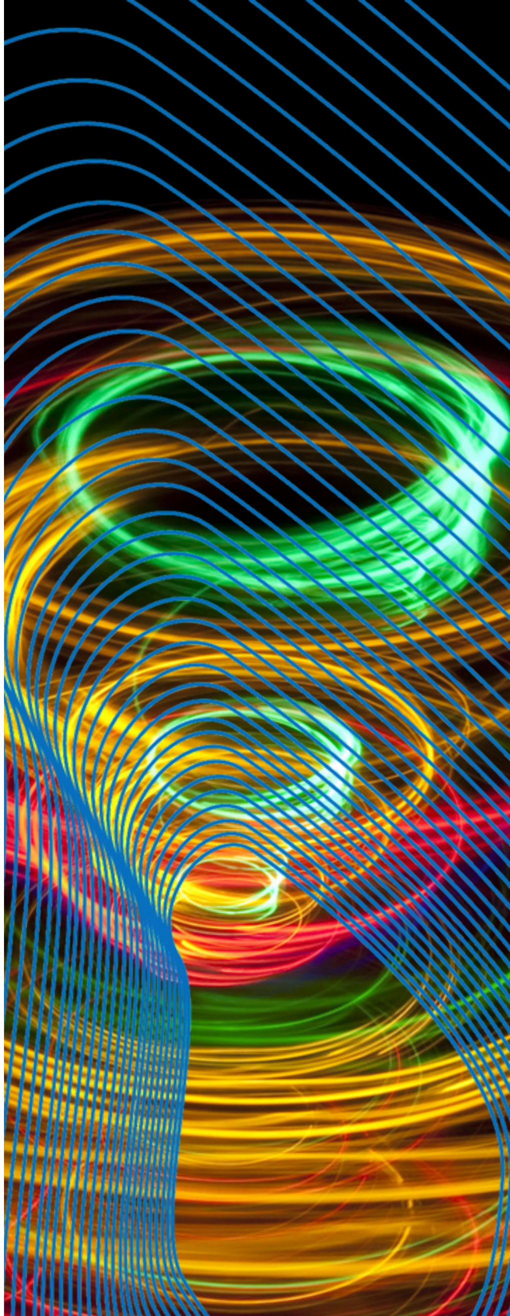

The quantum mechanical calculations require considerable computational power and were run on both national supercomputing facilities (ARCHER2) and STFC Hartree Centre's supercomputers. Approximately 1200 models (one per simulation) were built each comprising about 200+ atoms; each simulation used on average between 96 - 512 cores* for approximately 24 - 36 hours per simulation. The electrical energy consumed to carry out this research is a small fraction of the overall potential gain in energy efficiency offered by these spin-tuned spintronic devices should they eventually be manufactured.

*Equivalent to 12 to 64 powerful laptops