# KITE code could power new quantum developments

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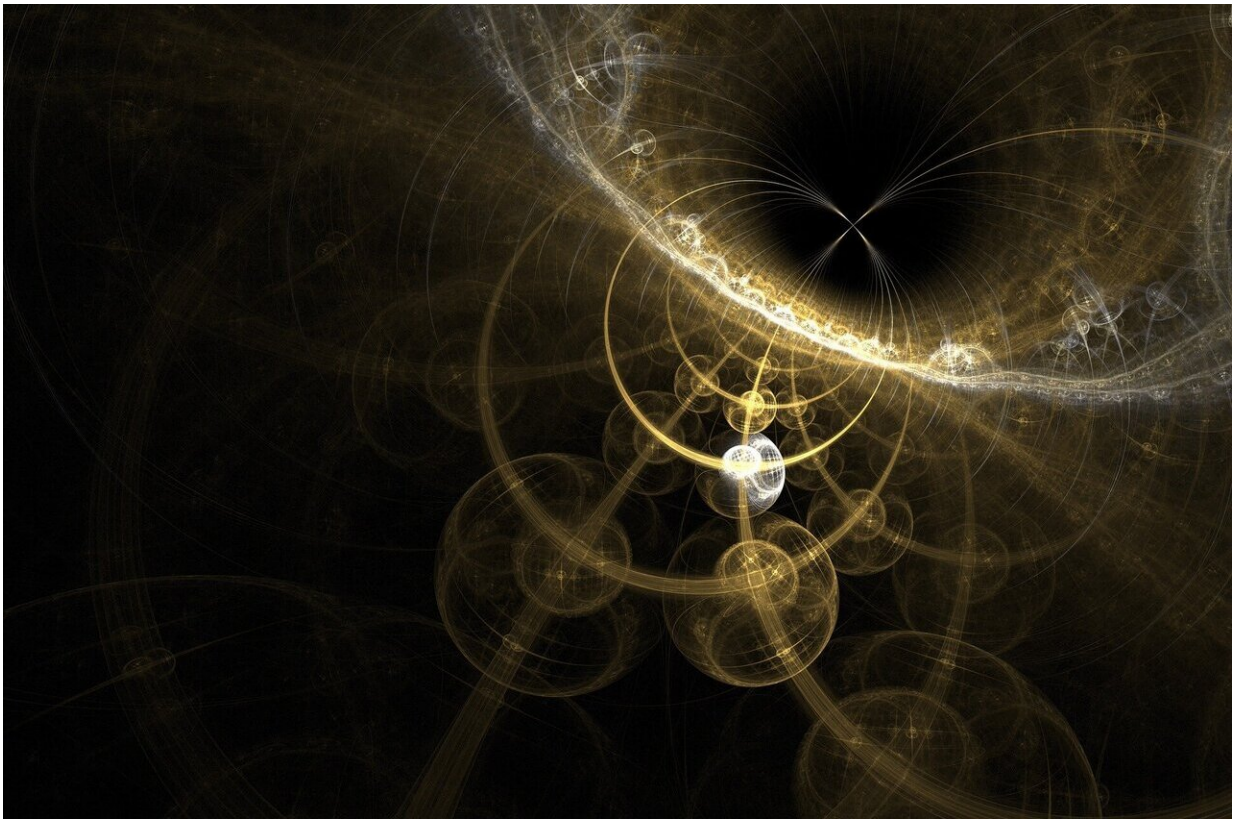

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A research collaboration led by the University of York's Department of Physics has created open-source software to assist in the creation of quantum materials which could in turn vastly increase the world's

computing power.

Throughout the world the increased use of data centres and cloud computing are consuming growing amounts of energy—quantum materials could help tackle this problem, say the researchers.

Quantum materials—materials which exploit unconventional quantum effects arising from the collective behaviour of electrons—could perform tasks previously thought impossible, such as harvesting energy from the complete solar spectrum or processing vast amounts of data with low heat dissipation.

The design of quantum materials capable of delivering intense computing power is guided by sophisticated computer programmes capable of predicting how materials behave when 'excited' with currents and light signals.

Computational modelling has now taken a 'quantum leap' forward with the announcement of the Quantum KITE initiative, a suite of open-source computer codes developed by researchers in Brazil, the EU and the University of York. KITE is capable of simulating realistic materials with unprecedented numbers of atoms, making it ideally suited to create and optimise quantum materials for a variety of energy and computing applications.

Dr. Aires Ferreira, a Royal Society University Research Fellow and Associate Professor of Physics, who leads the research group at the University of York, said:

"Our approach uses a new class of quantum simulation algorithms to help predict and tailor materials' properties for a wide range of applications ranging from solar cells to low-power transistors.

"The first version of the free, open source KITE code already demonstrates very encouraging capabilities in electronic structure and device-level simulation of materials.

"KITE's capability to deal with multi-billions of atomic orbitals, which to our knowledge is unprecedented in any area of quantum science, has the potential to unlock new frontiers in condensed matter physics and computational modelling of materials."

One of the key aspects of KITE is its flexibility to simulate realistic materials, with different kinds of inhomogeneities and imperfections.

Dr. Tatiana Rappoport from the Federal University of Rio de Janeiro in Brazil, said:

"This open-source software is our commitment to help removing barriers to realistic quantum simulations and to promote an open science culture. Our code has several innovations, including 'disorder cell' approach to simulate imperfections within periodic arrangements of atoms and an efficient scheme for dealing with RAM intensive calculations that can be useful to other scientific communities and industry."

Read the research paper in *Royal Society Open Science*.

**More information:** Simão M. João et al. KITE: high-performance accurate modelling of electronic structure and response functions of large molecules, disordered crystals and heterostructures, *Royal Society Open Science* (2020). DOI: 10.1098/rsos.191809

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