Largest molecular spin found close to a quantum phase transition

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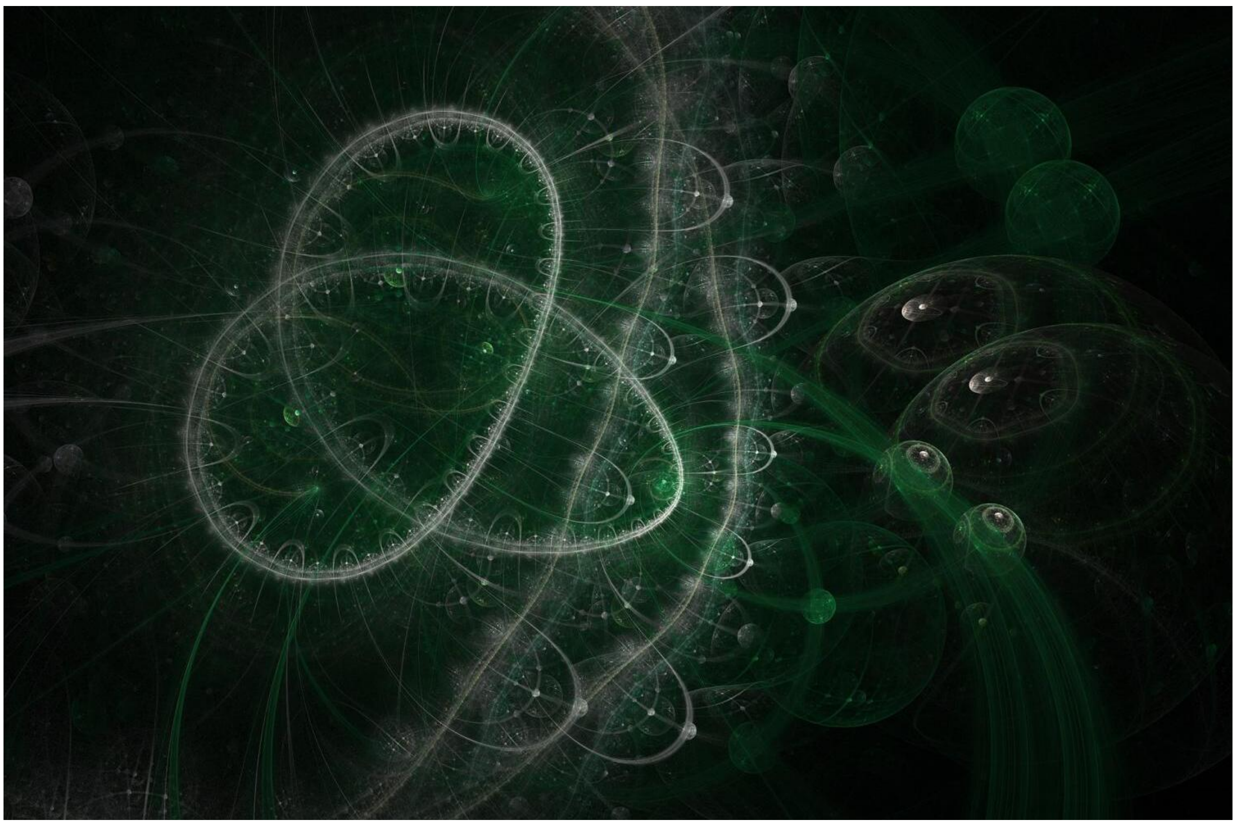

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An international research team headed by Professor Dr. Annie Powell, a chemist at the Karlsruhe Institute of Technology (KIT), and Professor Dr. Jürgen Schnack, a physicist at Bielefeld University, has synthesized a new magnetic molecule. The team has reported the largest ground state spin ever attained. It is publishing its new findings today (26.02.2018) in the new Nature partner journal *npj Quantum Materials*.

Every electron possesses a quantum mechanical intrinsic angular momentum, also called spin. The new magnetic molecule modelled at Bielefeld University and synthesized at the KIT reveals a spin in its ground state that is as large as that of 120 electrons combined. This makes it the largest spin ever observed in a single molecule. Magnetic molecules are molecules containing magnetic ions such as iron or gadolinium. The researchers report the synthesis of $Fe_{10}Gd_{10}$. It has the geometric structure of a torus.

Scientists in the interdisciplinary research project found a so-called quantum phase transition that strongly influences the property of the molecule. In quantum phase transitions, substances change their behaviour fundamentally at quantum critical points. An example of a 'classical' phase transition is that of water boiling as it passes a certain temperature. Quantum phase transitions occur at a temperature of absolute zero. In the newly synthesized $Fe_{10}Gd_{10}$ molecule, 10,000 states are degenerate at the critical point. That means they have the same energy. On this absolutely flat energy surface, it is possible to switch between the individual states without using any energy. In such a situation, the thermodynamic quantity entropy adopts giant values. "It's as if you were standing on top of a high pointed mountain," explains Annie Powell. "A small change to the external parameters, for example, to the pressure, suffices for it to immediately drop steeply." Therefore, future research will examine how external pressure can be used to lead the molecule $Fe_{10}Gd_{10}$ beyond the quantum critical point.

More information: Amer Baniodeh et al. High spin cycles: topping the spin record for a single molecule verging on quantum criticality, *npj Quantum Materials* (2018). DOI: 10.1038/s41535-018-0082-7

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