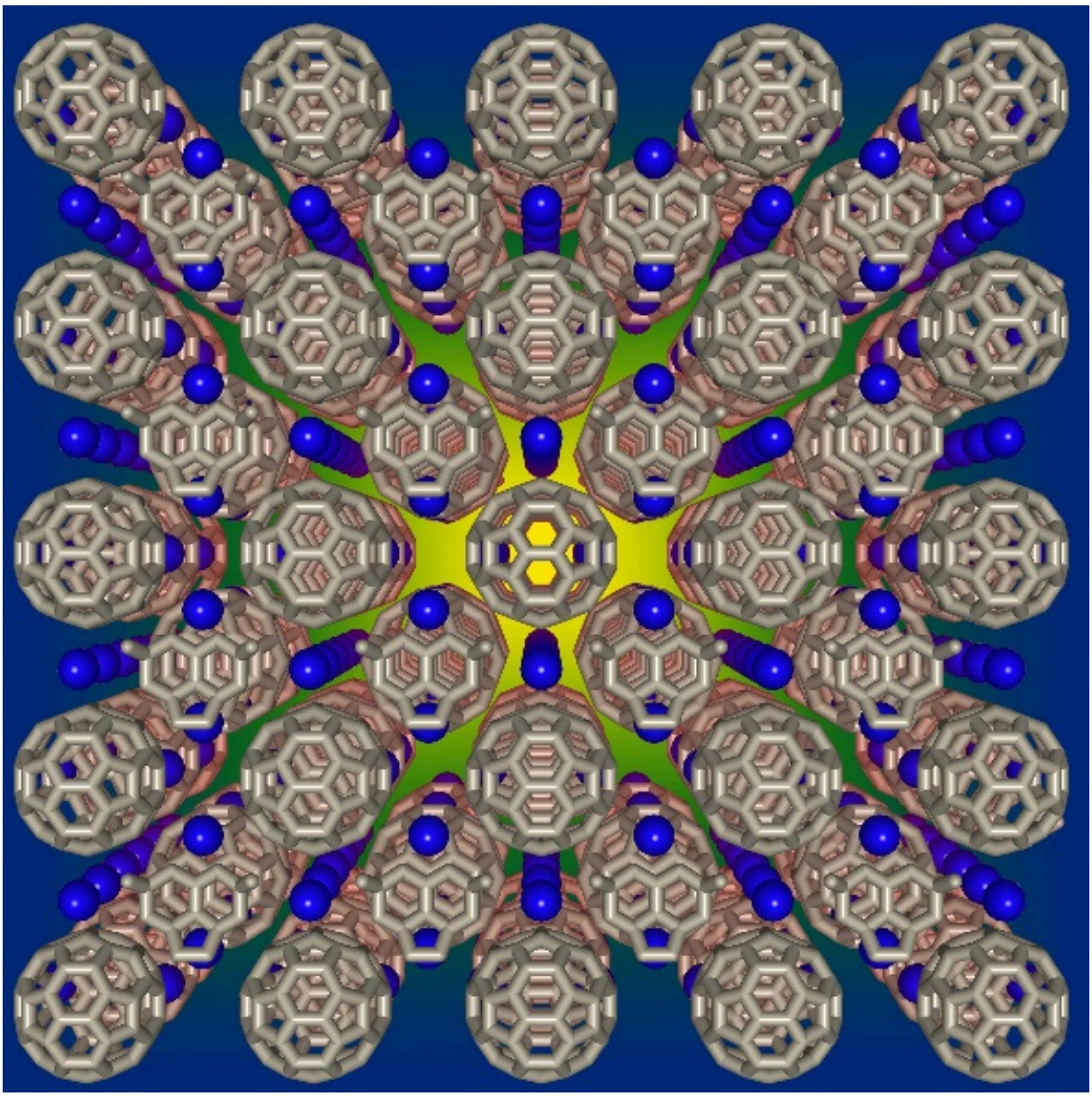
How to maximize the superconducting critical temperature in a molecular superconductor

April 17 2015



The fullerene molecules consist of 60 carbon atoms arranged in a truncated icosahedral shape (a soccer ball) and pack in a regular cubic-close-packed array in three dimensions. Alkali metal ions (blue spheres) occupy vacant interstitial holes of octahedral and tetrahedral symmetry. Credit: Prassides Kosmas

An international research team, led by Professor Kosmas Prassides of Tohoku University, has investigated the electronic properties of the family of unconventional superconductors based on fullerenes which have the highest known superconducting critical temperature (Tc) among molecular superconductors.

In results published in the American scientific journal *Science Advances*, the team was able to demonstrate the guiding influence of the molecular electronic structure in controlling superconductivity and achieving the maximum Tc, opening the way to new routes in the search of new molecular superconductors with enhanced figures of merit.

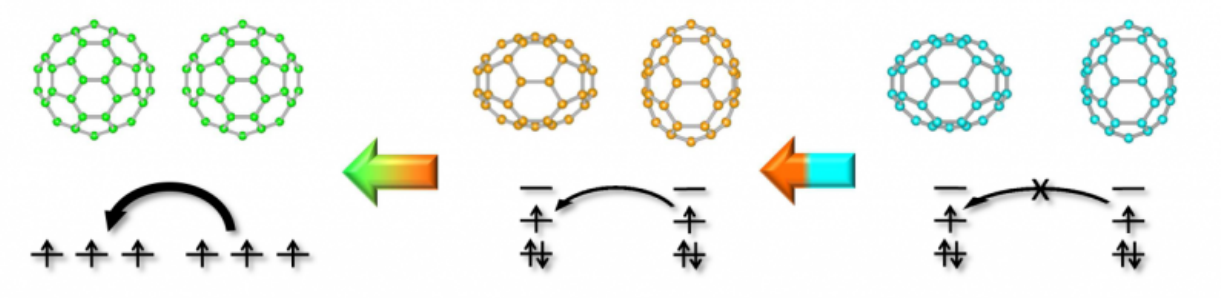
Background:

Metals are used for electricity transmission, but energy is lost as heat because of electrical resistance. Superconductors have no electrical resistance and can carry electricity without losing energy, so it is important to find superconductors which can work at the highest possible temperature.

Most superconductors have simple structures built from atoms. But recently, superconductors made from molecules arranged in regular solid structures have been found.

Work by members of the team on molecular fulleride-based systems has previously led to the discovery of the highest working temperature (at 38 K) for a molecular superconductor (*Nature Materials* 7, p. 367, 2008).

The electronic ground state, which is in competition with superconductivity, was found to be magnetically ordered (*Science* 323, p. 1585, 2009). And the zero-resistance superconducting state could be switched on by tuning the exact arrangement of the C60 molecules in the solid by external pressure (*Nature* 466, p. 221, 2010).



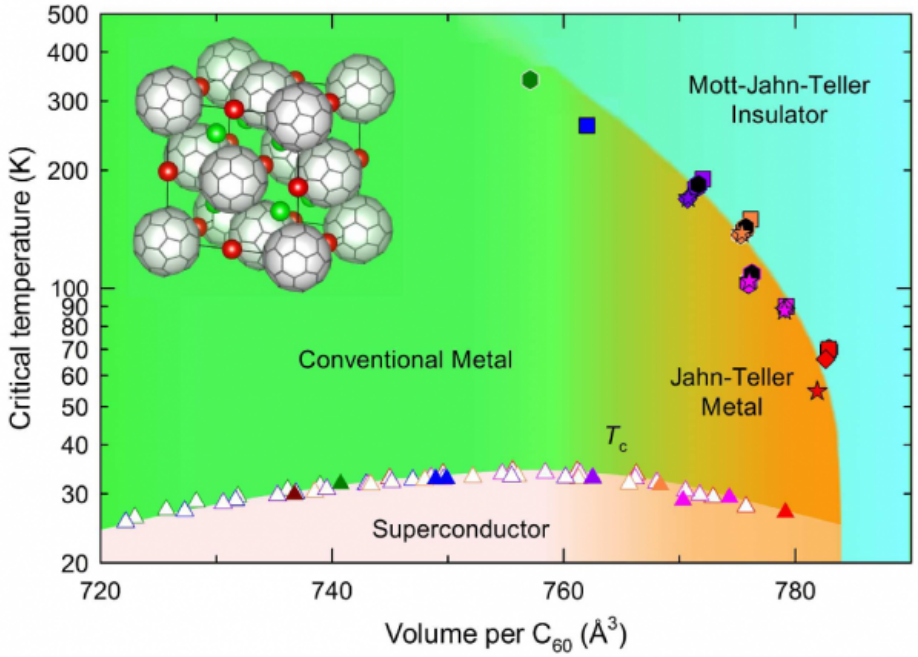
These are schematic depictions of the Jahn-Teller molecular distortion of the fullerene units in the Mott-Jahn-Teller insulator (blue molecules) and the Jahn-Teller metal (yellow molecules), their respective molecular electronic structure (lifting of the orbital degeneracy due to the distortion), and the resulting intermolecular hopping of the electrons (prohibited in the insulator, weak hopping in the Jahn-Teller metal). This situation contrasts with the behavior of the conventional metal where hopping is allowed, the orbital degeneracy is retained, and the molecules are undistorted (green molecules). Credit: Prassides Kosmas

The controlling role of the molecular electronic structure was then identified by demonstrating that the parent insulating state involves Jahn-Teller distortion of the molecular anions that produces the magnetism

from which the superconductivity emerges (*Nature Communications* 3, 912, 2012).

Breakthrough:

The research team has addressed for the first time the relationship between the parent insulator, the normal metallic state above Tc and the superconducting pairing mechanism in a new family of chemically-pressurized fullerene materials. This is a key question in understanding all unconventional superconductors including the high-Tc cuprates, the iron pnictides and the heavy fermion systems.



Electronic phase diagram of face-centered-cubic (fcc) structured fullerides

shows the evolution of the superconducting transition temperature, Tc (superconductivity dome) and the Mott-Jahn-Teller insulator to Jahn-Teller metal crossover temperature, T' as a function of volume per C60. Within the metallic (superconducting) regime, gradient shading from orange to green schematically illustrates the Jahn-Teller metal to conventional metal (unconventional to weak-coupling BCS conventional superconductor) crossover. The inset shows the crystal structure of fcc A3C60 fullerides (A=alkali metal, green spheres represent cations on tetrahedral and red on octahedral holes, respectively). Credit: Prassides Kosmas

Their work unveiled a new state of matter - the Jahn-Teller metal - and showed that when the balance between molecular and extended lattice characteristics of the electrons at the Fermi level is optimized, the highest achievable temperature for the onset of superconductivity is attained.

As synthetic chemistry allows the creation of new molecular electronic structures distinct from those in the atoms and ions that dominate most known superconductors, there is now strong motivation to search for new molecular superconducting materials.

More information: *Science Advances*, vol. 1, article number: e1500059, 2015 . DOI: 10.1126/sciadv.1500059

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