Weakly bonded salt is a key ingredient for high-purity Li@C60 film

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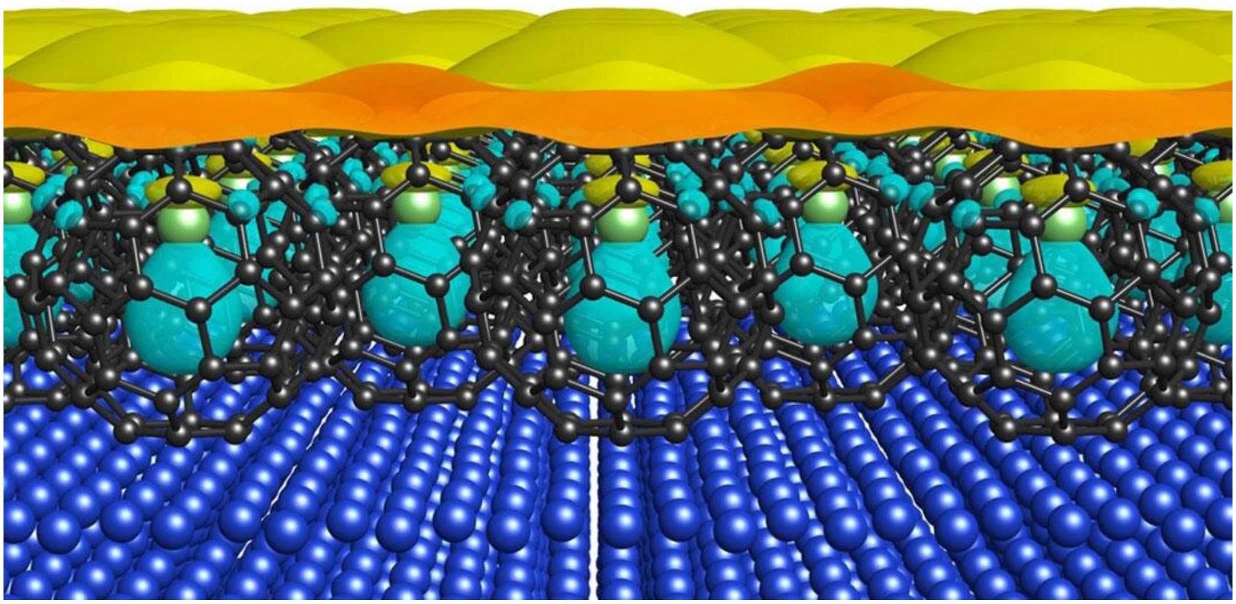

Researchers from the University of Tsukuba successfully grow a Li@C60 film on a copper surface to study the molecular orbitals. Credit: University of Tsukuba

As well as making it one of the most widely recognized molecules, the distinctive soccer ball shape of C_{60} gives it some useful properties. One of which is thought to be electrical conductivity when multiple molecules are close together. Efforts have therefore been made to optimize C_{60} so that it can be applied to electronic devices. Now, researchers at the University of Tsukuba have devised a way of depositing films based on C_{60} to provide a robust model to study. Their findings are published in The *Journal of Physical Chemistry Letters*.

Organic electronics—based on carbon atoms—offer advantages such as being cheaper, lighter, and more flexible than traditional metal alternatives. They are therefore expected to play a big part in the future of electronics.

C_{60} is a promising organic electronic material that has been further optimized by including a lithium ion inside the cage to give $Li@C_{60}$. If a layer of lithium filled cages can be arranged close together on a surface, the molecular orbitals of these structures—known as superatom molecular orbitals (SAMOs)—are thought to be sufficiently diffuse and overlapping to allow them to transport electrons.

Attempts have been made to prepare $Li@C_{60}$ films to study by depositing them from salts. However, the heat required caused the lithium ions to be dislodged, leaving many of the C_{60} cages empty. The researchers used a salt with a larger, less strongly bound anion, which meant lower temperatures could be used and a monolayer of intact $Li@C_{60}$ could be formed.

"Although our previous efforts to deposit $Li@C_{60}$ films gave us the opportunity to study single superatoms, we didn't get the complete picture we were looking for," explains study corresponding author Professor Yoichi Yamada. "Using the $[Li@C_{60}]\ NTf_2–$ salt produced a stable monolayer and provided us with an excellent opportunity to study the SAMOs."

The researchers used scanning tunneling microscopy and density functional theory calculations to study the Li@C_{60} film. They found that although the s-SAMO was localized on the individual Li@C_{60} molecules, the pz-SAMO was much more diffuse, allowing the transport of electrons.

"We have demonstrated a successful model that will be useful for future Li@C_{60} monolayer experiments," says Professor Yamada. "And although we are not quite at the stage of making electronic devices based on Li@C_{60} a reality, our findings provide a significant step in the right direction."

More information: Naoya Sumi et al, Direct Visualization of Nearly Free Electron States Formed by Superatom Molecular Orbitals in a Li@C60 Monolayer, *The Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/acs.jpclett.1c02246

Provided by University of Tsukuba

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