Visualization of molecular soccer balls

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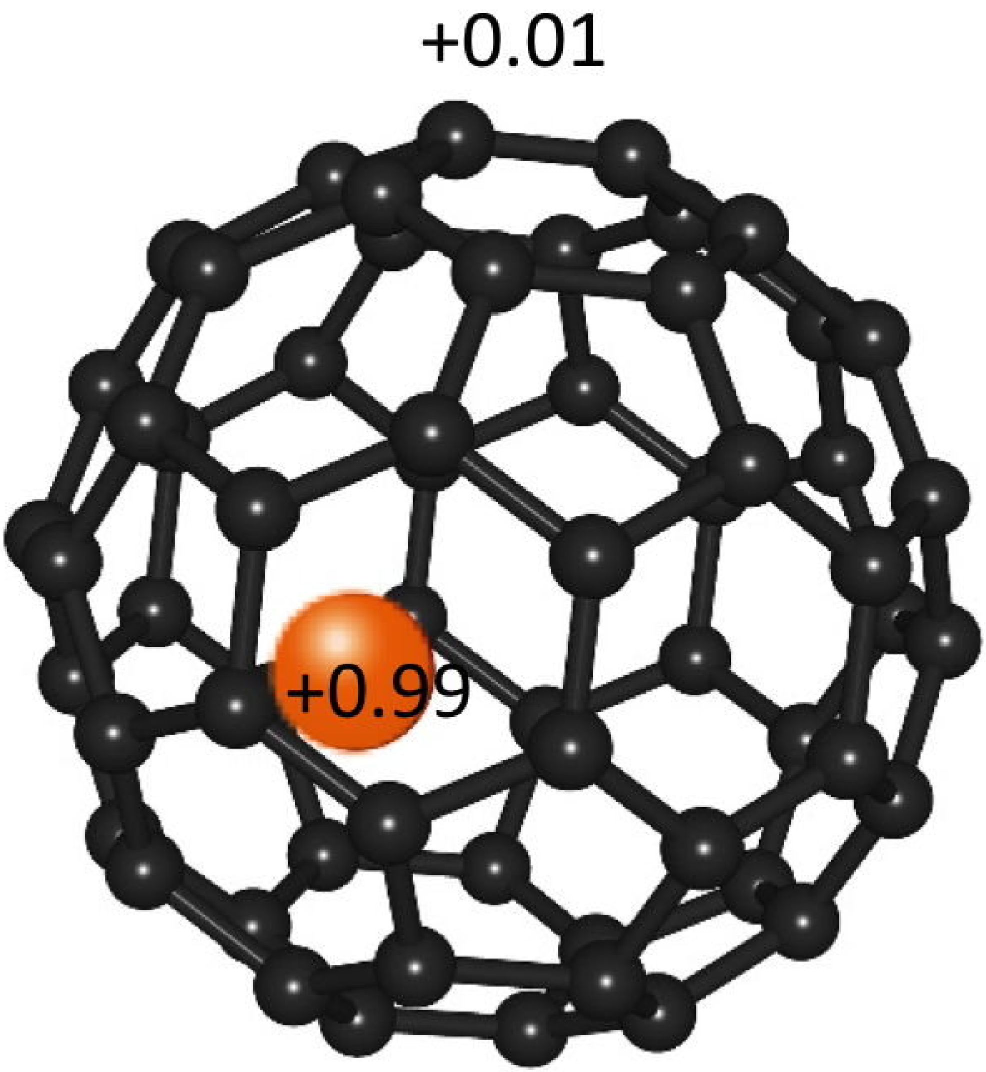

Calculated geometry and charges of LiþC60[PF6 -] salt. Credit: University of

Tsukuba

Fullerenes are composed of 60 carbon atoms joined together in hexagonal rings to form a sphere that resembles a soccer ball. Fullerenes are of great interest to materials scientists because their interesting electronic properties make them attractive for use in advanced electronics and nanotechnology.

The electronic properties of fullerene can be modified by doping with other elements without altering its soccer-ball shape. In particular, salts of lithium ion-doped fullerene, which is denoted as $Li+@C_{60}$, have been synthesized in high yield, and the structure of $Li+@C_{60}$ has been determined. $Li+@C_{60}$ salts have been used in solar cells and molecular switches with promising results.

To optimize the performance of $Li+@C_{60}$ in applications such as photovoltaics and switching devices, it is important to thoroughly understand its electronic properties. An international research collaboration led by the University of Tsukuba recently expanded knowledge of $Li+@C_{60}$ by imaging single $Li+@C_{60}$ molecules via scanning tunneling microscopy (STM). STM can image materials with molecular-level resolution and provide information about the electronic structure of single molecules. The results were published in the journal *Carbon*.

"We fabricated a thin-film sample suitable for STM by vacuum evaporation of a $Li+@C_{60}$ salt on a copper substrate," says study co-author Seiji Sakai. "Our subsequent microscopy examination revealed that although some lithium ions escaped during the evaporation process, the sample did contain some $Li+@C_{60}$ molecules on the copper substrate."

The microscopy images revealed a mixture of Li+@C_{60} and undoped fullerene molecules on the copper surface. Both types of molecules were similarly oriented but displayed different heights and electronic structure, allowing them to be differentiated. The team lent further weight to their experimental findings by conducting density functional theory calculations to generate simulated scanning tunneling microscopy images. The experimentally measured and simulated microscopy images agreed well overall.

"Our study provides confirmation of the electronic structure of lithium-doped fullerene," lead author Yoichi Yamada says. "Such knowledge will aid our ability to modulate the electronic structure of fullerenes to optimize their performance in optoelectronic and switching devices."

The imaging and electronic structure confirmation of Li+@C_{60} represent important steps toward advanced applications of organic materials, because they should contribute to controlling the carrier injection and transport properties of fullerenes.

More information: Yoichi Yamada et al, Electronic structure of Li + @C 60 : Photoelectron spectroscopy of the Li + @C 60 [PF 6 −] salt and STM of the single Li + @C 60 molecules on Cu(111), *Carbon* (2018). DOI: 10.1016/j.carbon.2018.02.106

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