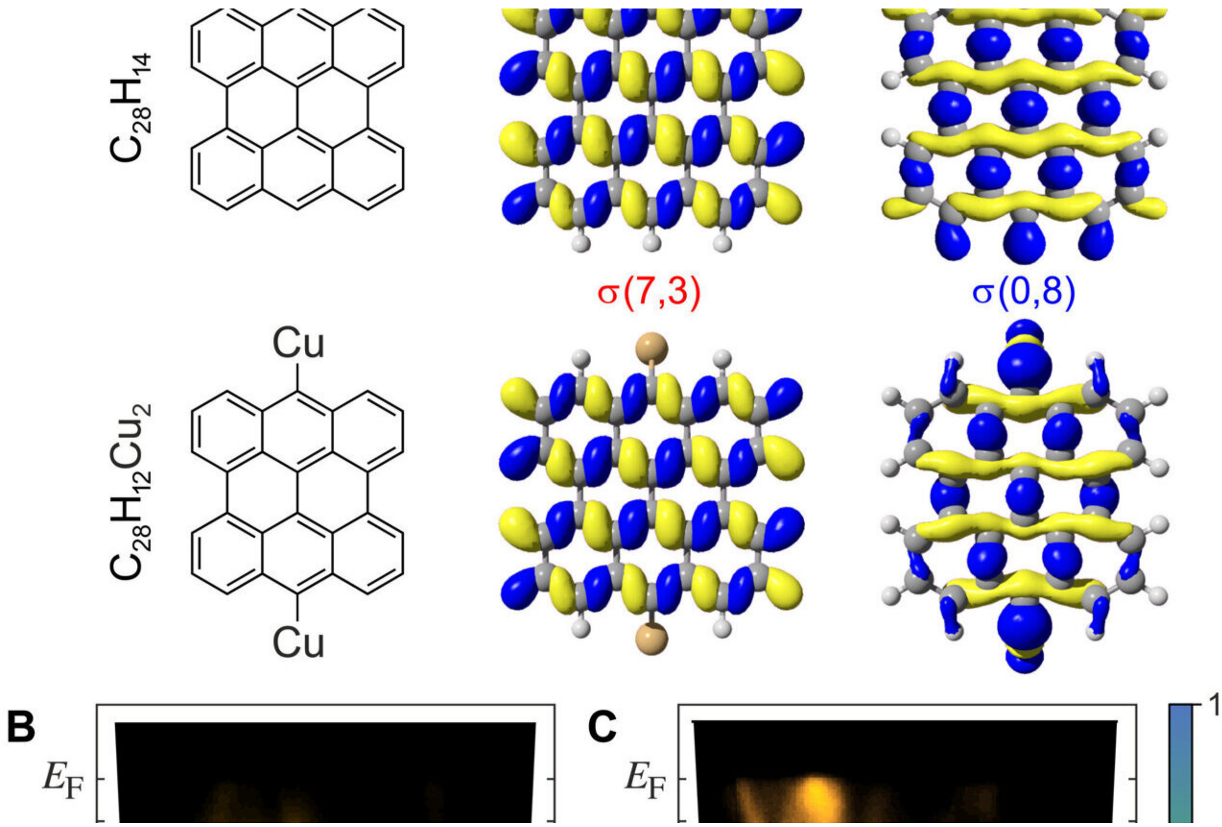
Testing shows photoemission orbital tomography can detect sigma orbitals

August 4 2022, by Bob Yirka



σ orbitals and ARPES band maps. (A) σ(7,3) and σ(0,8) orbitals of bisanthene (C28H14, 4) (top) and metalated bisanthene (C28H12Cu2, 5) (bottom). (B and C) Band maps along the [11¯0] and [001] directions. π and σ bands are labeled. The white dashed lines denote binding energy Eb of the k∥ map in Fig. 4A. Credit: *Science Advances* (2022). DOI: 10.1126/sciadv.abn0819

A team of researchers affiliated with several institutions in Germany and Austria reports that it is possible to use photoemission orbital tomography to detect σ orbitals. In their paper published in the journal *Science Advances,* the group describes modifying one aspect of photoemission orbital tomography to make σ orbitals visible.

For many years, chemists and physicists have been working toward mapping the sphere that exists around atomic nuclei—within such spheres, there are shells that define the areas where electrons are likely to exist at any given time, with each given a name, such as σ or π.

For many years, researchers have used scanning tunneling microscopes to better understand the structure of atoms, most particularly the depth of a given electron's potential well. The approach is only likely to work for a limited number of shells, mostly in π orbitals. Because of that, researchers have looked for other ways to study the shells.

In 2009, a group of researchers developed a new approach called photoemission orbital tomography. It involved shining ultraviolet light on a surface and then measuring the energies (and angles) of the electrons that were knocked out due to the photoelectric effect. The technique was used to map π orbitals, but problems arose when trying to use it to map σ orbitals. Still, researchers believed it should work—they even found a way to prove it mathematically. In this new effort, the researchers found a way to circumvent the earlier problems, allowing for the technique to be used with σ orbitals.

The approach used in the new effort involved applying synchrotron radiation. This expanded the energy range used in the photoemission orbital tomography process. But adding such an energy source created another problem: how to measure the results. To solve that problem, the team developed a custom program that analyzed data from the tomography process and provided a detailed analysis of the σ orbitals.

The researchers found that the spectra were close to predictions, and the results also answered unresolved issues in surface chemistry science. They next plan to see if their method can be used in real time.

More information: Anja Haags et al, Momentum space imaging of σ orbitals for chemical analysis, *Science Advances* (2022). DOI: 10.1126/sciadv.abn0819