Functionalizing Molecular Nanocarbon with Fluorine Atoms

Antonio Moreno-Vicente[1], Marc Mulet-Gas[2], Paul W. Dunk[2], Josep M. Poblet[1], Antonio Rodríguez-Fortea[1]

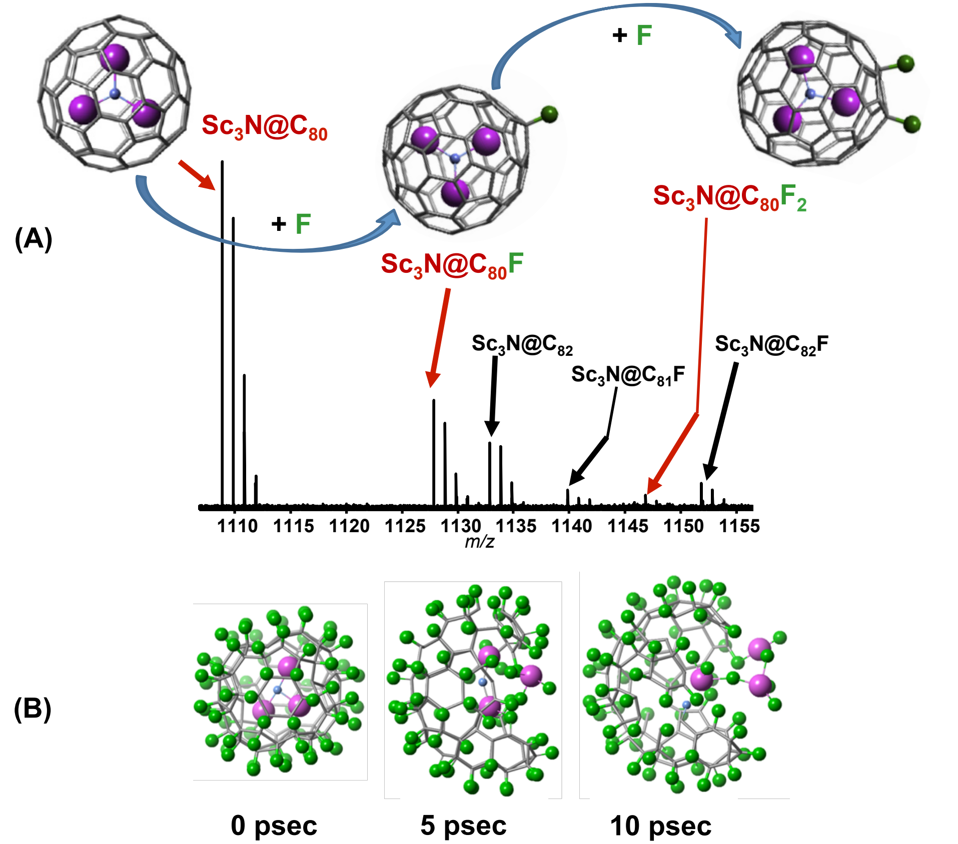
1. University of Rovira i Virgili, Spain; 2. National High Magnetic Field Laboratory, Florida State University

Funding Grants: G.S. Boebinger (NSF DMR-1157490, NSF DMR-1644779); A. Rodríguez-Fortea, J.M.Poblet (MCI CTQ2014-52774-P, GC 2014SGR, and XRQTC)

Endohedral metallofullerenes (EMFs) contain metal-based clusters (e.g., Sc_3N) within the nanoscale void of their C_{80} cages. Their exceptional properties have gained intensive interest for potential applications in biomedicine and photovoltaics. For example, water-soluble EMFs are powerful MRI contrast agents. Also, the addition of a fluorine atom to the cage chemically tunes nanomaterials for use in plastic solar cell technology, technology that converts sunlight into clean energy.

MagLab users from Spain have used laser-based chemical sampling techniques in the MagLab's Ion Cyclotron Resonance (ICR) facility to develop the synthesis of fluorinated molecular nanocarbon. The addition of fluorine (F) to the $Sc_3N@C_{80}$ compound has been an elusive goal, because all prior attempts have destroyed the fullerene cage. In this work, the researchers discovered a route that uses widely available and cheap polytetrafluoroethylene, more commonly known as Teflon, to selectively add one or two F atoms to the cage.

This research demonstrates that high field ICR mass spectrometry combined with theoretical calculations can unleash the discovery of new carbon compounds for sustainable energy, as well as shed light on fundamental behaviors of carbon nanoforms.



(A) Up to two fluorine atoms are added to the $Sc_3N@C_{80}$ fullerene cage, as shown in the FT-ICR mass spectrum. **(B)** Calculations show that too many fluorine atoms (shown in green) destroy the cage (i.e., the cage opens after five picoseconds), whereas the controlled addition of only one or two fluorine atoms, as discovered in this work, keeps the nanocage intact.

Facilities and instrumentation used: Ion Cyclotron Resonance, 9.4 T actively shielded magnet, cluster instrument

Citation: A. Moreno-Vicente, M. Mulet-Gas, P.W. Dunk, J.M. Poblet, A. Rodríguez-Fortea, *Probing the formation of halogenated endohedral metallofullerenes: Predictions confirmed by experiments*, **Carbon** 129, 750-757 (2018)