Pressemitteilung

Freie Universität Berlin
Christine Xuan Müller

30.04.2025
http://idw-online.de/de/news851396

Wissenschaftliche Publikationen
Biologie, Chemie
überregional

Overcoming the “Fluoro Wall” Researchers observe tunneling effect of heavy atoms for the first time

An international research team made up of scientists from Freie Universität Berlin and the French National Center for Scientific Research (CNRS) in conjunction with Université de Lorraine in Metz, France, has achieved a significant breakthrough in the chemistry of fluorinat-ed compounds. With the aid of quantum chemical simulations they were able to prove for the first time that heavy fluorine atoms can also “tunnel,” or in other words, transform be-tween two states. The study “Experimental Observation of Quantum Mechanical Fluorine Tunneling” was published in the scientific journal Nature Communications.

It opens up new prospects for controlling chemical reactions and understanding better what makes certain fluorinated compounds particularly stable or reactive.

Fluorine and fluorinated compounds are commonplace in our everyday lives. Fluorinated groups improve the uptake of medications in the body; fluorinated compounds make cell-phone batteries more efficient and allow them to last longer; and fluoride in toothpaste pre-vents cavities. At the same time, per- and polyfluoroalkyl substances (PFAS) pose a growing problem for human health and the environment.

Extensive research on the science behind the interactions produced by fluorine and its com-pounds is needed in order to fully grasp both the positive and negative effects of fluoride in compounds. This is one of the objectives of the Collaborative Research Center (CRC) 1349 “Fluorine-Specific Interactions,” which has been funded by the German Research Foundation (DFG) since 2019. Within the framework of CRC 1349, teams led by Professor Sebastian Ha-senstab-Riedel and Professor Beate Paulus from Freie Universität Berlin together with Pro-fessor Jean Christophe Tremblay from the French National Center for Scientific Research (CNRS) in conjunction with Université de Lorraine in Metz, France, have now discovered a unique fluorine-specific interaction.
Over a decade ago Hasenstab-Riedel and his team managed to capture an unusual molecule in a neon crystal at -270°C. This molecule – an anion comprised of just five tightly packed, highly charged, and unstable fluorine atoms – should not actually exist. And yet, the mole-cule remained surprisingly stable.

In order to understand what held this molecule together, researchers in Paulus’ team to-gether with Tremblay carried out extensive calculations and quantum mechanical simula-tions. They came across a surprising effect that had up to this point mainly been observed for hydrogen, which is very light, but which was considered virtually impossible for the relatively heavy fluorine atom. The researchers were able to prove that even fluorine atoms can effec-tively tunnel – i.e., make a molecule spontaneously transform between two states that are actually separated by a finite energy barrier. This type of tunneling has already been observed in other molecules of much lighter ele-ments such as hydrogen and oxygen. Until now, researchers assumed that fluorine atoms were too heavy to tunnel at all, which is why they tended to speak of a “fluoro wall” when it came to tunneling.

However, this new study appears to signify a paradigm shift. The combination of special bonding conditions in molecules that are trapped in a very small space seems to make it possible for atoms that are heavier than oxygen to tunnel. "The findings don't just expand our understanding of chemical bonds in fluorinated compounds," says Dr. Carsten Müller of Freie Universität Berlin, first author of the study. "They have also provided us with new tools to control molecular reactions in a targeted manner – whether that is in materials research, medicine, or designing new technologies."

wissenschaftliche Ansprechpartner:

Dr. Carsten Müller, Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Email: carsten.mueller@fu-berlin.de
Prof. Dr. Sebastian Hasenstab-Riedel, Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Email: s.riedel@fu-berlin.de

Originalpublikation:

https://www.nature.com/articles/s41467-025-59008-6

URL zur Pressemitteilung: http://More information on Collaborative Research Center (CRC) 1349 "Fluorine-Specific In-teractions": https://www.sfb1349.de/en/index.html