Better insight into molecular interactions

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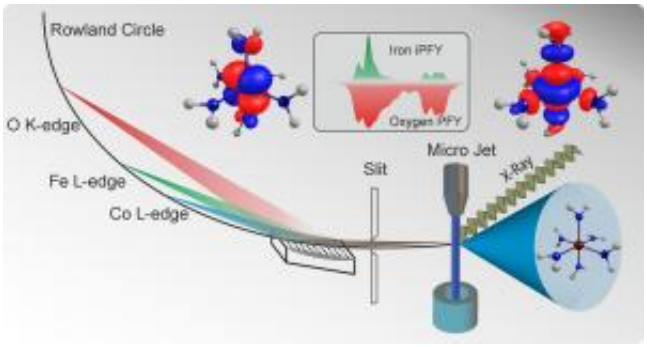

This sketch demonstrates the principle of measurement which enables to address atom-specific and state-dependent emission of photons. With the help of first principles theory the spectral features can be associated with molecular orbitals. Credit: Uni Rostock

How molecules in biochemical solutions do interact, is a question of great importance for understanding processes in catalysts, functional materials and even in organisms. Until now, scientists could have a look at these interactions by spectroscopy, but it was hard to distinguish the different interactions, which take place simultaneously. A groundbreaking work by HZB-scientist Emad Flear Aziz and theoretical physicist Oliver Kühn from University Rostock could now change the game.

The results are published in *Physical Review Letters*.

"Basically we are looking at how atoms and molecules interact in

biochemical materials in solution", says Professor Dr. Emad Flear Aziz, leader of the Young Investigator Group for Functional Materials in Solution at the HZB and Professor at Freie Universität Berlin. Their now published work is based on a discovery by Aziz' team made three years before: They then analyzed samples with x-ray spectroscopy and observed the disappearance of photons at some specific photon energy. These results have been replicated by other teams worldwide. To explain this effect, Aziz and colleagues proposed a "dark channel mechanism", which should provide information about binding processes and interactions between atoms or molecules. This explanation stirred a big debate among scientists.

Now they have gathered arms with theoretical physicists around Professor Oliver Kühn from the University of Rostock in order to get a coherent picture: Aziz' team sharpened the experimental methods further using a new approach to high resolution spectroscopy. In order to understand, how the spectral findings are linked to binding and structural processes inside the sample, Oliver Kühn and his postdoc Sergey Bokarev provided a theoretical tool, based on ab initio calculations of energy levels inside the molecules. "We can map all electronic states in the systems we probe, and we can distinguish those which are involved in building bonds with neighbors from those which are not involved", Aziz explains. Metaphorically speaking: if the interacting molecules produce a sort of party chatter, the scientists are now able to listen to specific conversations. They are convinced that these new tools will bring deeper insights into the chemistry of life.

More information: "State-Dependent Electron Delocalization Dynamics at the Solute-Solvent Interface: Soft-X-Ray Absorption Spectroscopy and Ab Initio Calculations" *PRL*, DOI: 10.1103/PhysRevLett.111.083002