PRESS RELEASE

Oxygen: Bond breaking in a jumpy way

HZB is involved in researching quantum beating, which expands our knowledge on the creation and destruction of chemical bonds.

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Breaking the bond between two atoms is an elementary step in a chemical reaction. The atoms separate until they feel no more interaction. It turns, if one of the atoms comes close enough to another atom, then it can be captured by it, resulting in a new chemical bond. The quasi-classical prevailing notion of this process is that the atoms continuously move apart: When a bond breaks, the atoms can be found at any distance alike.

An international team of scientists, with the involvement of Professor Dr. Alexander Föhlisch and Dr. Justine Schlappa of the Institute 'Methods and Instrumentation for Synchrotron Radiation Research' at Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) has shown that this notion has to be revised: When oxygen molecules break apart, for example, the atoms are not found at all distances, but only at few selected ones.

The scientists made this discovery when they illuminated gaseous oxygen with synchrotron light. This light led to an excitation of the oxygen molecules, where the chemical bond between the two oxygen atoms in the molecule were temporarily broken. The researchers measured the light scattered back from the molecules and gained information about the distance of the oxygen atoms at specific times. The scientists chose the energy of the incident light such that the dissociation process could take place in two ways. The only distinction between these two ways was that the separating atoms were moving at different speeds.

The results of their measurements showed that the distances at which oxygen atoms were detectable had preferential values: In other words, there are distances during bond breaking at which the oxygen atoms prefer to remain, and other places where they were not found. To explain this phenomenon, HZB scientist Dr. Justine Schlappa draws an analogy with a slightly out-of-tune guitar: "If a musician plucks two notes on the strings at slightly shifted frequencies to each other, then he hears the sound go periodically louder and quieter. Acousticians call this rise and fall in volume "beating". It disappears

Dr. Justine Schlappa

Photo: HZB

when the instrument is perfectly tuned and the frequencies of the tones are perfectly harmonized."

The cause for this beating is the inherent wave characteristic of sound. "When the waves of two tones are slightly shifted relative to each other, this results in interference," says Schlappa: "Wave crests that occur simultaneously reinforce each other and the sound becomes louder. If wave troughs encounter wave crests, however, then they cancel each other out – the sound becomes quieter." Just as with sound, the physicists now regard the behaviours of separating oxygen atoms as waves. Justine Schlappa continues: "The two possible speeds at which the oxygen atoms can separate leads to the slightly shifted frequencies in the oxygen waves and cause the so-called quantum beating." Again, wave crests reinforce one another and there are locations in space where atoms are preferentially found. Wave crests and wave troughs cancel each other out with the result that there are locations where no atoms reside.

"Our observation has profound consequences for our understanding of chemical reactions," says Professor Dr. Alexander Föhlisch, head of the HZB institute 'Methods and Instrumentation for Synchrotron Radiation Research'. "If no atom can be detected, then no other chemical steps can take place at that distance," Föhlisch continues. "This is a serious limitation for the pathways of chemical reactions and forces us to rethink our idea of chemical processes from the ground up."

A. Pietzsch et al., Spatial Quantum Beats in Vibrational Resonant Inelastic Soft X-ray Scattering at Dissociating States of Oxygen, Phas.; Rev. Lett. 153004 (2011).
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