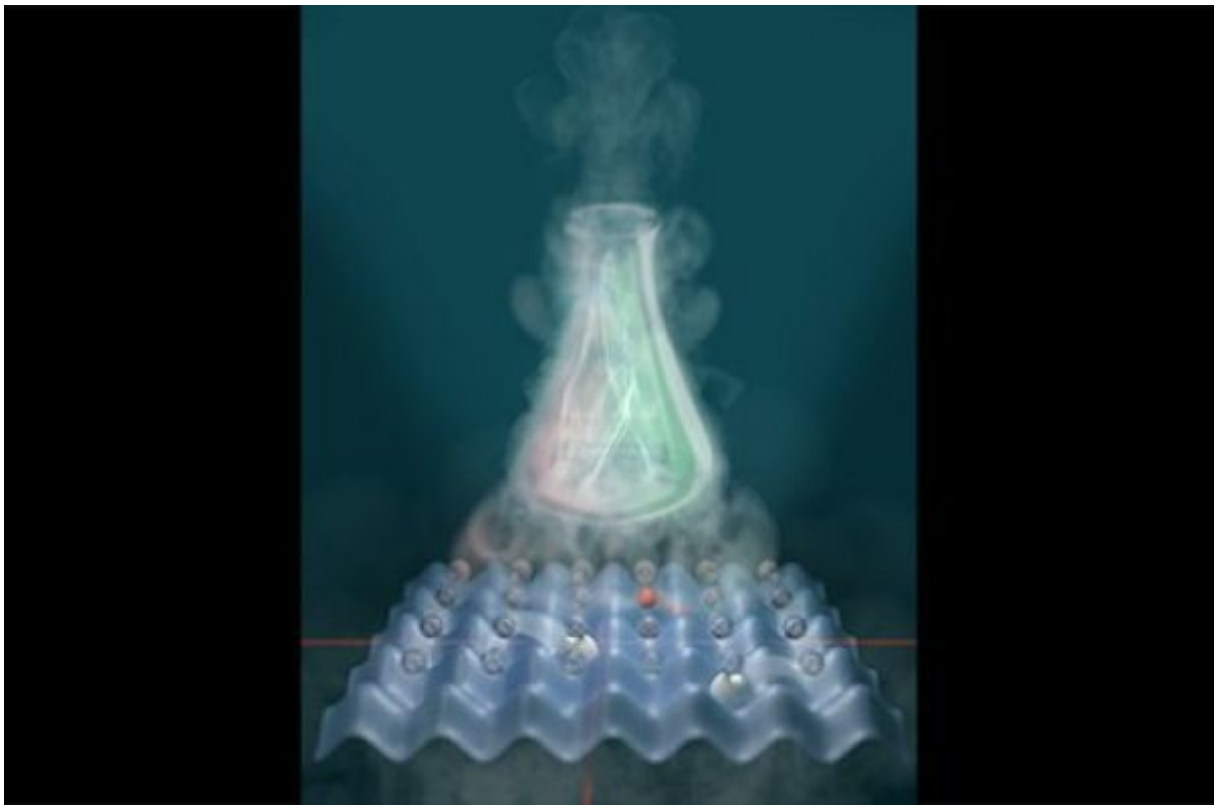

Simulating molecules with quantum simulators

A study published in Nature provides a solution on how to simulate chemical reactions with quantum chemistry.

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Being able to simulate how a molecule unfolds or how it reacts with another one to produce a larger molecular compound is an extremely complex task. So far, classical computers or even supercomputers have not been able to model the many-body interactions that occur within such compounds, simply because they do not have the capacity to process this information in a reasonable amount of time.

As a solution, quantum simulators have become an alternative approach to tackle quantum problems that overpass our computational capabilities. In particular, they have been used in the field of condensed matter physics and to imitate crystals but, until now, it remained unknown how to simulate the interactions between electrons accurately enough within complex molecular systems.

Thus, in a study recently published in Nature initiated at MPQ in Garching, researcher Javier Argüello-Luengo, currently a doctoral candidate at ICFO, together with Alejandr Gonzalez-Tudela from IFF-CSIC, Tao Shi from CAS, Peter Zoller, Director of IQOQI, and led b Ignacio Cirac, Director and Head of the Theory Department at the MPQ, report on a ne approach that shows how an analog quantum simulator could mimic the quantum chemistr of molecules.

In their quantum simulator, they use a regular, three-dimensional atomic lattice, which can be created by several intersecting laser beams, the "optical lattice". The intersection points can form an egg carton shape into which the atoms are filled. The interaction between the atoms can then be controlled by amplifying or attenuating the rays.

In the proposed theoretical model, electrically neutral atoms in the optical lattice assume the role of electrons. The atoms can move freely from well to well in the "egg carton", similar to the electrons in the shell of a real molecule. The challenge is now how to mimic the way in which electrons interact with each other, effect known as Coulomb interaction. In particular, simulating the repulsion between each other because they have the same electrical charge. This effect can be observed even over long distances. However, the atoms in the "egg carton" only interact with their direct neighbours.

Thus, to describe this Coulomb interaction, the scientists looked back into their quantum theory books. According to this, electrons repel each other by exchanging a light particle (photon). In a similar manner, the new approach suggests the following. First, each well in the "egg carton" is filled with additional atoms. Each of these atoms can be energetically excited by the irradiation of a laser light, providing the medium for transmitting the interaction. An excited background atom passes the energy on to its neighbour, who passes it on to its neighbor and so on and so forth. The excitation moves around like a photon through the medium. The "electron" and the excited background atom repel each other. If the excitation that travels around meets the second "electron", the repulsion occurs as well. This is how the effect is mediated. The probability for such an exchange decreases with the distance between the two "electrons", as it does with the Coulomb interaction.

The results of the study prove this approach as a plausible option to simulate larger molecules than hydrogen. As Javier Argüello-Luengo mentions, "Our work now opens up th possibility of efficiently calculating the electronic structures of molecules using analogu quantum simulation. This will trigger a richer understanding of the (bio)chemistry problem that are hard to explore with today's computersi¿½.