Micrometer-size molecular modeling kit shows real chemical reactions

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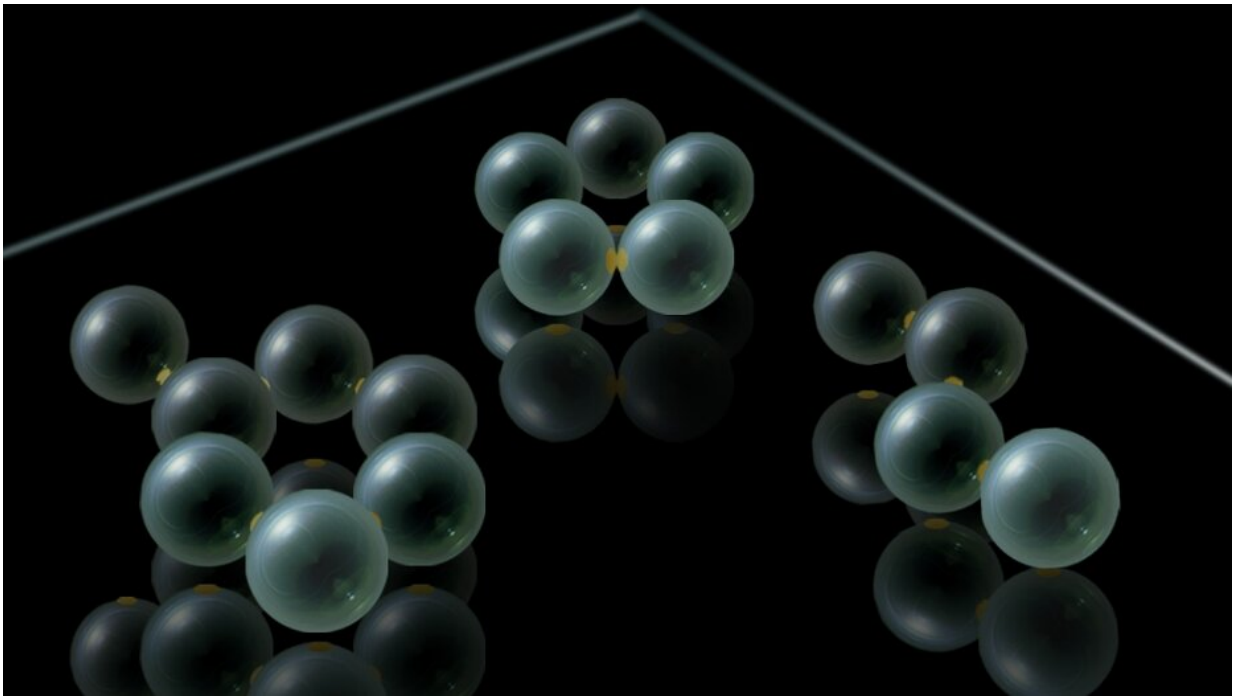

An artist's impression of some molecules that can be made and studied using the new modelling kit. Credit: Laura Quarto

Molecules are so small that we cannot even see them with ordinary microscopes. This makes studying molecules or chemical reactions difficult: researchers are limited to either indirect observations or computer models. A team of researchers from the University of Amsterdam and New York University have now found a way to build

micrometer-size model molecules using 'patchy particles'. This allows for a much more direct study of molecular dynamics. The results were published in *Nature Communications* this week.

When we learn chemistry in high school, we use molecular modeling kits in which the atoms are represented by wooden or plastic balls that you can connect to form molecules. These modeling kits help us to visualize the spatial structure of molecules and imagine how they react, but obviously no real chemical reactions occur between the wooden or plastic balls. It now turns out that for very small balls this situation changes dramatically.

A new modeling kit

While molecular modeling kits can be very useful, most of our actual knowledge about molecules arises in a much more indirect way. It comes, amongst others, from measurements of the spectrum of radiation that the molecules absorb. For instance, an infrared spectrum provides scientists with a fingerprint of the molecular vibrations from which they can deduce the molecular composition and structure. Adirectviewof molecules would allow immediate insight into their arrangement, molecular vibrations and reactions. However, such direct images are precluded by the molecules' small size and fast motion. The fact that all observations of molecules are indirect, challenges our imagination of the three-dimensional molecular structures and reactions.

This issue led physicists and chemists of the University of Amsterdam and New York University to find a way to combine the easy visualization of common molecular modeling kits with the actual physics that goes on at the sub-nanometre scale of real molecules. In the laboratories in Amsterdam, the scientists managed to build "molecules" from small micrometer-size plastic balls, so-calledcolloidal particles, that were produced in the New York labs. The particles were made in such a way

that they attract each other in certain directions only, modeling very precisely the specific angles between chemical bonds between atoms, which determine the way in which the atoms arrange into molecules.

These micrometer-size particles indeed combine the best of both worlds: they are small enough to exhibit the characteristic motion and vibrations that molecules experience due to temperature, but are just large enough to be observed and followed using a regular microscope.

Atoms in, molecules out

To imitate specific types of atoms, the researchers in Amsterdam used techniques that were developed over the past few years to equip the colloidal particles with attractive patches where the model atoms could 'click' together. The number and configuration of these patches determines the type of atom that is modeled—for example, to imitate carbon atoms, the researchers made particles with four patches in a tetrahedron geometry, or particles with two patches on opposite sides, reproducing the bond angles of two well-known binding states of carbon atoms. On top of that—and this is where the new kit goes far beyond common molecular models—they managed to finetune the interactions between the patches so that the model atoms were able to form bonds and split up again in the exact same way that atoms do in real chemical reactions.

The modeling kit turned out to work excellently. When several model atoms were brought together, the researchers observed that the particles indeed formed the "molecules" that are well known from carbon chemistry. Under a microscope, analogs of molecules such as butyne and butane were visible—molecules that have their main atoms arranged along a line. Molecules with ring-like configurations, which play an important role in organic chemistry, could also be modeled: structures such as cyclopentane (a molecule with a ring of five carbon atoms) and

cyclohexane (with a ring of six such atoms) could be observed.

Puckering and catalysis

Due to the larger size of the model molecules, the researchers could follow their formation and internal motion in real time and in great detail. This allowed them to directly see phenomena that were only known to occur from indirect observations. For example, for the five-atom ring structure of cyclopentane, they directly observed the characteristic "puckering" motion of the constituent atoms: the cyclopentane ring is not fixed in a single plane, but it deforms so that constituent atoms move in and out of that plane. The reason for this behavior is that the natural angles between the atoms do not exactly match the angles that are needed to make a flat five-atom ring, and as a result one atom always has to be puckered out of the plane. So far, the resulting puckering motion had only been observed by indirect spectroscopic measurements, but now the researchers were able to see it happen before their very eyes, following the motion directly in real space and time. They found that the flips occurred collectively: the up- and down motion of a particle influenced that of all other particles in the ring.

Using the same molecule, the researchers could then observe how chemical reactions took place. The ring was observed to open up and attach to other molecules—an effect which could be strengthened by adding an attractive surface to the setup. That is, the surface acted as a catalyst, providing insight—quite literally—into what happens during such catalytic reactions.

Small enough yet large enough

Of course, the micrometer-size of the model atoms is still a factor of

1000 or so larger than the sub-nanometre size of actual atoms, but the point is that they are small enough to undergo random thermal motion, and this is what makes chemical reactions happen. As Richard Feynman famously put it in his lectures, "Everything that living things do can be understood in terms of the jigglings and wigglings of atoms"; and it is precisely these jigglings and wigglings, clearly observable when looking at the colloidal atoms with a microscope, that distinguish the micrometer-size molecular modeling kit from its counterpart that we know from high school.

Thus, the modeling kit is a very useful tool to directly observe "molecules" in their natural habitat, and should have many useful applications. Besides giving an attractive visualization of molecules, the results provide insight into the action of geometric catalysts on molecular reactions. Furthermore, the availability of the new small building blocks opens the door to the design of complex new materials, directly under the microscope, with a host of applications ranging from artificial tissue for e.g. medical purposes to functional nanostructures that can be used in technology.

More information: P. J. M. Swinkels et al. Revealing pseudorotation and ring-opening reactions in colloidal organic molecules, *Nature Communications* (2021). DOI: 10.1038/s41467-021-23144-6

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