Dive into the world of molecules

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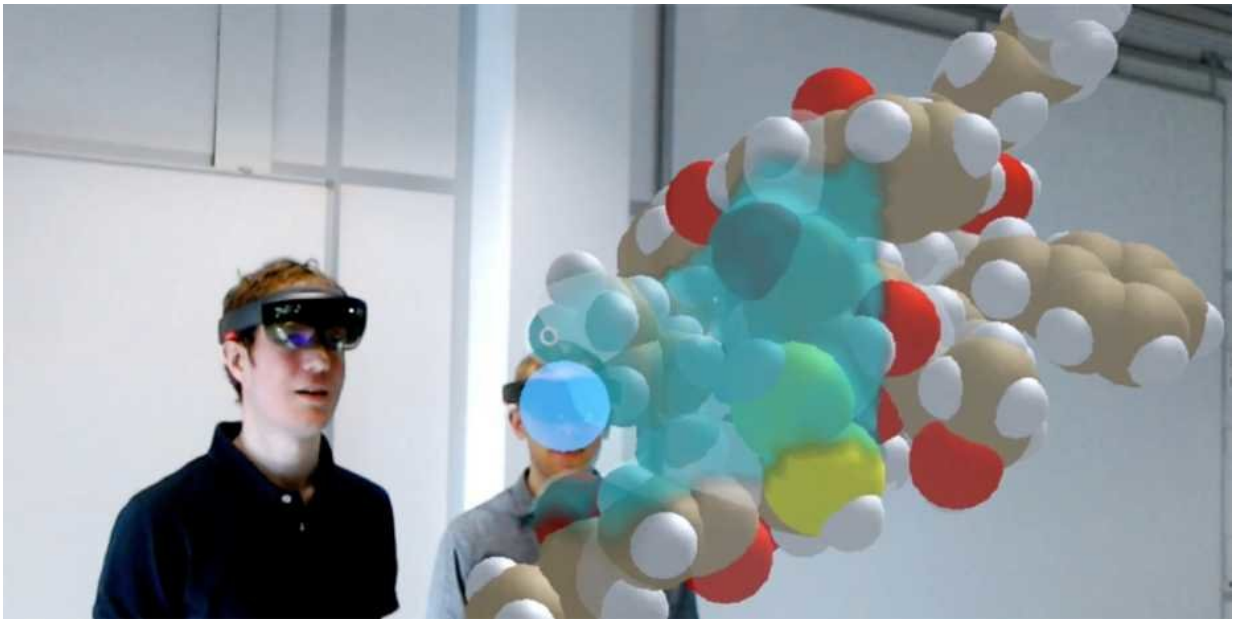

By using HoloLens glasses, a protein can be experienced as a virtual object in space. Credit: ETH Zurich

Brand new technology in the classroom: students immerse themselves in a "mixed reality" and use HoloLens glasses to learn a fundamental principle of proteins.

From the outside, it looks like a futuristic meditation exercise. In reality, it's part of the Computer-Assisted Drug Design course run by Gisbert Schneider, Professor in the field of the same name. In this case, reality has two components – the glasses worn by the students convey a mixed

reality.

Anyone who looks through the HoloLens, as the glasses produced by Microsoft are called, not only sees the furniture and people present in the room, but also a hologram. In Schneider's course, the virtual object is a protein that the students can walk around, investigate and even walk through.

Using the HoloLens in practice

The glasses are being put to use in a two-week practical course, during which the students experience a condensed version of the whole cycle of active drug ingredient development. The first week focuses on theory: "Among other things, the students learn how to screen a catalogue of millions of molecules to separate out the ones that could interact with a particular protein thanks to their form and function," explains Schneider. At the end of the first week, the students are split into small groups. Each group is now a virtual company that has to develop an inhibitor for a protein.

Next, the students conduct a screening themselves and have to decide on one or two molecules out of the ones they find. In the second week, they go into the laboratory to synthesise the molecule and test its activity. At the end of the week, they have to sell it as a company.

Understanding the protein's structure

"To find a suitable molecule, the students have to have an understanding of the protein's surface, and particularly of which cavities the molecule could fit into," explains co-course leader Jan Hiss. Developing this understanding is not so easy. The surface of a protein is defined by the position of the atoms it is made up of. The individual atoms have a Van der Waals radius that is specific to each atom. These radii result in a

spherical model of the protein. "For example, if you move a water molecule over this spherical model of the protein, a new surface will be produced. Its form depends on where the water molecule touches it," says Hiss, explaining the principle of the solvent-accessible surface. He uses the HoloLens to visually illustrate this principle after he has taught the students the theory.

"With the HoloLens, the students can immerse themselves in the protein, almost like a water molecule themselves," says Hiss of the experience. They can not only look at the protein, but also produce the solvent-accessible surface themselves by moving the water molecule as a virtual probe over the protein's surface. In this way, the students can see why they are not able to reach certain sites on the protein.

Further potential applications

This innovative learning project stemmed from a call for suggestions on the use of HoloLens in teaching from ETH Zurich's Educational Development and Technology department (LET). Thanks to a donation by ETH alumnus Adrian Weiss, LET was able to purchase twelve of these glasses, which are currently finding an enthusiastic reception not only in the entertainment industry, but in business more widely.

As the technology is still brand new and uses are still very much experimental, the company Afca offered to develop a first teaching application. The concept submitted by Hiss convinced LET, and so Afca used his idea to develop the app called Molegram.

With Molegram, ETH's teaching has taken its first step into the world of mixed reality. And there will be plenty more to come: in a second project, geomatics students are programming their own apps for HoloLens. And LET has already put out another call for project suggestions.

Provided by ETH Zurich