RETHINKING DESIGN

ETH Zurich Meets Davos during the World Economic Forum's Annual Meeting (22 – 25 January 2019)

Information, photographs, and video footage

Drug Design – Inside Molecules

Zurich, 15 December 2018

Often perceived as more art than science, "Drug Design" the graphical representation of molecular structures strongly inspires the development of drug therapies. Molecular models make visible a world otherwise invisible to the naked eye. They enable and facilitate our understanding of the molecular world. Based on these graphical models, a chemist can identify potential drug binding sites on the surface of a protein, understand molecular interactions between a drug molecule and its "target", and design novel drugs that will eventually become medical therapies.

Any model represents only parts of the true nature of things. Therefore, it is helpful to consider multiple models and graphical representations simultaneously. Visualizing three-dimensional objects on a computer screen by creating the illusion of three-dimensionality has certain limitations. Here, holographic models provide a potential solution. At the ETH Zurich Pavilion in Davos during the 2019 World Economic Forum, we present the MOLEGRAM Explorer for the holographic visualization of this exciting molecular nanoworld.

The MOLEGRAM Explorer provides a fresh view on molecules to both experts and non-experts alike. The user can fully submerge him or herself into the topic by physically circling and investigating the hologram of a protein structure. In the Computer-Assisted Drug Design practical class at ETH Zurich, the participants use this application to examine and interact with a protein and learn the influence of different solvents on the protein structure.

The application, designed for a 15-minute usage, includes an introductory movie on the Hololens hardware. The MOLEGRAM Explorer enables collaborative learning by providing a real-time synchronized view of the hologram to all participants. A shared pointer allows the instructor to focus the participants' awareness on certain areas of the protein. The application also offers the "Explorer mode" allowing the students to apply the new concept in an individualized environment.

We invite you to discover the holographic molecular world with us!

References

Dive into the world of molecules, ETH Zurich News article
https://www.ethz.ch/en/news-and-events/eth-news/news/2018/02/hololens.html

Hololens Goes Education
http://www.cadd.ethz.ch/education/hololense.html

Computer-Assisted Drug Design at ETH Zurich
http://www.cadd.ethz.ch/

Bios / publications

Gisbert Schneider, Professor of Computer-Assisted Drug Design / Institute of Pharmaceutical Sciences at ETH Zurich
http://www.cadd.ethz.ch/people/gisbert_Schneider.html

Petra Schneider, Institute of Pharmaceutical Sciences at ETH Zurich
http://www.cadd.ethz.ch/people/dr-petra-schneider.html

Jan Hiss, Institute of Pharmaceutical Sciences at ETH Zurich
http://www.cadd.ethz.ch/people/jan_Hiss.html

Images and video material

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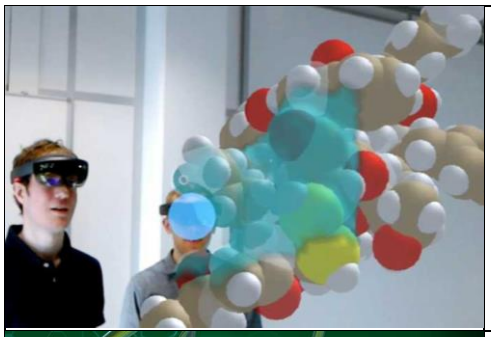

Drug Design:
ETH Zurich students use Microsoft's HoloLens to explore molecules in virtual reality

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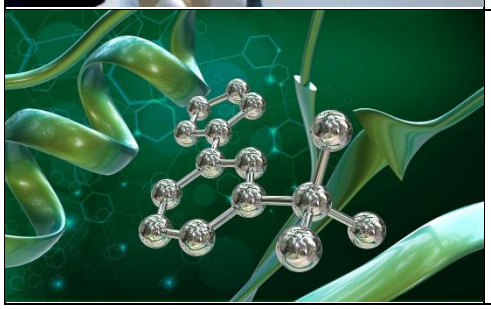

Exploring Molecular Structures
Understanding molecules and their structures inspires chemists to identify potential drug binding sites on the surface of a protein.

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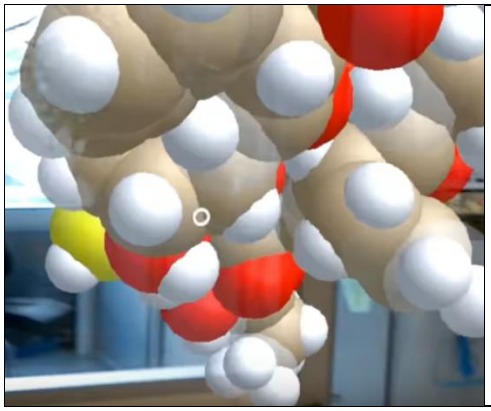
Background Information



Video:
Students immerse themselves in a “mixed reality” using Microsoft’s HoloLens to learn fundamental principles of proteins. Prof. Gisbert Schneider uses the HoloLens in a Computer-Assisted Drug Design course at ETH Zurich

https://youtu.be/Ihick-4aLw0