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Chemical Education

A CHIMIA Column

Topics for Teaching: Structural Chemistry and Biology

Updates on moleculARweb, the Swiss Portal for Chemistry and Structural Biology Education Using Augmented and now also Virtual Reality

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Abstract: We present a new activity on the moleculARweb platform on molecular symmetry elements, two more languages, a new marker-less augmented reality mode, and a new virtual reality tool for VR headsets.

Keywords: Augmented reality · Education · moleculARweb · STEM · Technologies

Among the most interesting and engaging tools to assist STEM education, there are augmented reality (AR) and virtual reality (VR), especially in commodity forms, *i.e.* that run on regular devices such as smartphones, tablets and laptops, or on VR headsets in the low-hundred dollars.[1–3]

Our main contribution in the field of AR/VR tools for STEM is moleculARweb, a free-to-use platform intended to make learning about chemistry and structural biology more interactive and engaging by means of web apps that exploit commodity AR[4] and VR.[5] Each web page inside moleculARweb offers an AR-based activity or playground where users can manipulate virtual objects that represent atoms, molecules and other entities relevant to various fields of chemistry and biology, by presenting pairs of fiducial markers to the webcam.[6] By moving the markers in space, users can control the orientation and position of up to two objects at a time, thus enabling their seamless inspection in 3D in an intuitive manner and triggering of interactive content -such as molecules moving, clashing, or interacting with each other.

The content available at moleculARweb covers a range of topics arranged in five main modules: (i) one containing playgrounds with versatile tools to load and display any molecule or object,[7] and others dedicated to (ii) orbitals and molecular shapes, (iii) hydrogen bonding, including acids and bases, (iv) the atomistic structure of biological macromolecules, and (v) large biological assemblies.[4]

In this short column we present the latest updates to moleculARweb, including new activities, modes, and features.

The main update in the content is the addition of a new activity on symmetry elements for 12 molecules that illustrate the main point groups. This activity allows users to visualize the different symmetry elements of a molecule, such as rotational axes and planes of symmetry, in an interactive and engaging way. Understanding how rotations and reflections alter (or do not alter) the configurations of atoms in molecules requires strong efforts in abstract 3D visualization. With this new tool, students and teachers can selectively toggle on and off the display of all symmetry elements for the 12 molecules on two independent markers (Fig. 1). Hopefully, this tool will facilitate the teaching and understanding of symmetry aspects.

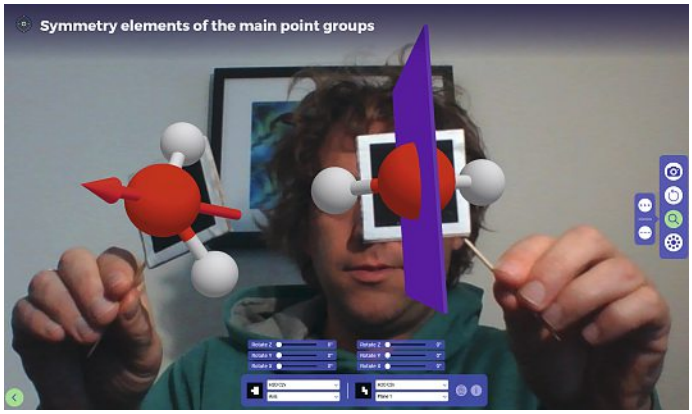

Fig. 1. The new activity on symmetry elements. Here, the user holds models of water molecules with a C_2 symmetry axis shown on the left and with one of the symmetry planes on the right. The person holding the markers in the field of view is author LAA.

The other important update is a playground implementing a new marker-less mode with access to all the static objects from the whole website. This new playground, which works for the moment on laptops and computers only, allows users to explore augmented reality content without the need for fiducial markers. Instead, the tool directly tracks the user's hands, providing in principle a more intuitive and immersive experience as compared to the use of marker-based tracking (Fig. 2). In this tool, hand tracking in the browser is achieved through the Mediapipe library.[8] This library can take around one minute to load, and is more computationally demanding than marker tracking. Still, we think it is important to offer this mode because it is the starting point for a potential evolution of the whole website in which all interactions take place directly with bare hands. This can be achieved at high performance with modern VR headsets,[5] but these devices are not affordable in most countries, hence developing ways to manipulate molecules with bare hands right on computers is of major interest.

For even deeper, more immersive experiences, moleculARweb now counts with a new playground ('Build your own WebAR views') that allows users to create VR experiences for absolutely any molecule in PDB format or 3D object exported from the VMD program. As explained in detail in our technical article,[5] after processing a molecular structure or VMD object with this tool the user receives an e-mail with multiple links to launch the generated scenes. One of them is the VR mode, that runs smoothly in any VR headset equipped with a WebXR-enabled web browser (we have verified proper functionality in

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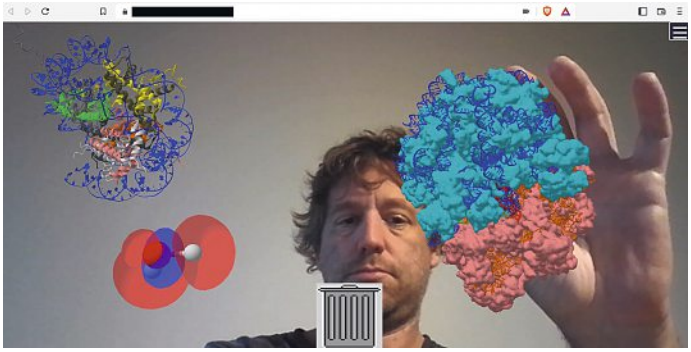

Fig. 2. The new playground for marker-less object manipulation. Here, the user has loaded 3 objects that remain 'floating' and can be grabbed and manipulated with the hands (here from left to right: a PDB structure of a nucleosome, a water molecule with a molecular orbital, and a cryo-EM structure of a ribosome). The person in the field of view is author LAA.

Oculus Quest, Quest 2, Quest Pro, and HTC Vive Pro headsets). Fig. 3 shows example applications shot from inside an Oculus Quest 2, with videos linked in the caption.

Another important update in moleculARweb is the addition of translations of Thai and Russian, allowing the site to cater to an even wider audience, now in eight languages. In the roadmap, we plan to include some more systems of biological interest and a chatbot for on-the-fly, 24-7 consultations through natural conversation.

The over 60,000 visits to moleculARweb since its launch in 2020 and the sustained visits over time by people from all over the world, attest to its wide adoption (Fig. 4). We hope that the new material and updates presented here will serve to further improve educational experiences and make the whole content of the website more accessible, as we pursue to provide fun, engaging ways to learn about chemistry and structural biology.

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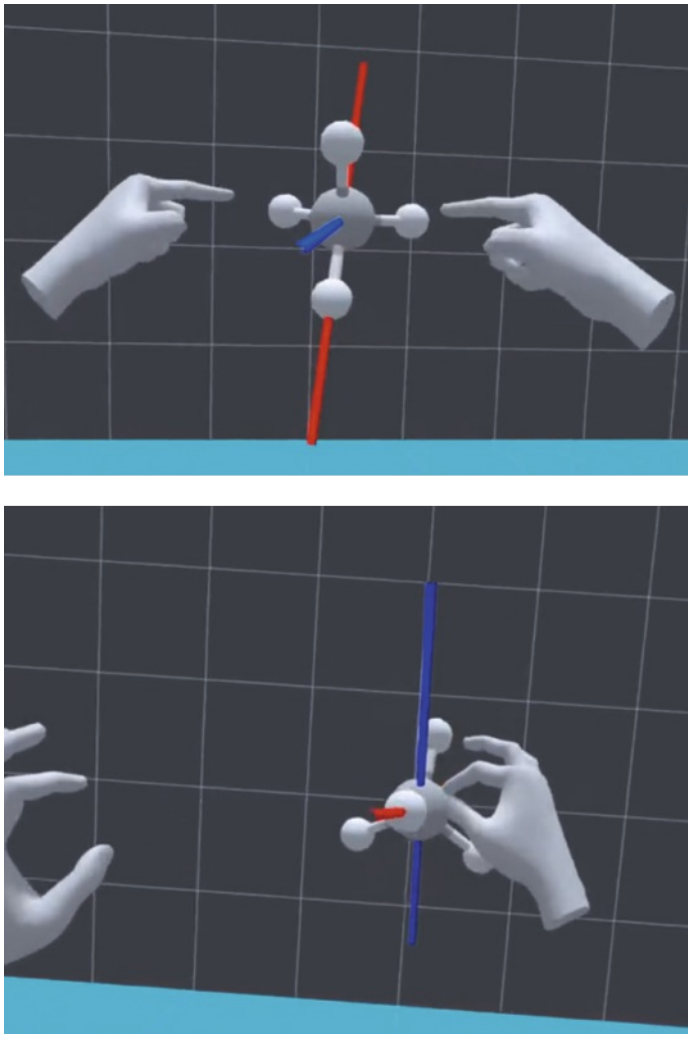

Fig. 3. Handling 3D objects in immersive VR. The example, produced with moleculARweb's new tool 'Build your own WebAR views' and seen here inside the web browser of an Oculus Quest 2 VR headset, depicts a VMD-generated model of methane with examples of its C_2 (blue) and C_3 (red) symmetry axes. See accompanying video of this specific example at https://twitter.com/i/status/1517819305982926849. Readers can test this VR example at https://molecularweb.epfl.ch/pdb2ar/methane/vr/.

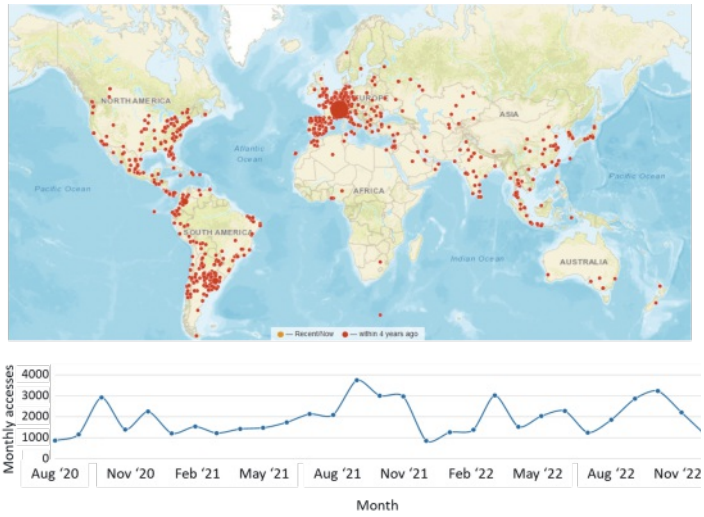

Fig. 4. Worldwide usage of moleculARweb since its release. All this data can be consulted right online at https://clustrmaps.com/site/1ar2f.