Virtual-reality view on chemistry and materials science

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We present a multi-platform tool that allows us to explore materials in Virtual Reality (VR) which has been developed within the Novel Materials Discovery (NOMAD) Laboratory, a European Centre of Excellence (https://nomad-coe.eu). The so far implemented functionality covers (Fig. 1) crystal structures, Femi surfaces, molecular-dynamics trajectories, and electron-hole pairs (excitons). The latter are 6-dimensional objects where VR can show its potential to visualize effects that otherwise are hard to capture. We demonstrate the power of our implementation on the large variety of data from the *NOMAD Repository*, *Archive*, and *Encyclopedia* which host several millions of calculated materials properties. We will give a life demonstration of molecular adsorption on surfaces and excitons in an organic-inorganic hybrid material.

Our platform can be utilized to view various types of datasets commonly used in chemistry and materials science. The tools run on various state-of-the-art VR setups – from extremely low cost to extremely high cost, adjusting the rendering quality according to the equipment. Our goal is to offer the system that suits the users' budget and needs best. This may range from Google Cardboard (a few Euro) to smartphone-based Samsung GearVR (order 200 Euro) and PC-based HTC-Vive (order 1000 Euro) to room-sized CAVE-like[i] equipment (order Mio. of Euro).

The project received funding from the European Union's Horizon 2020 research and innovation program under grant agreement no. 676580 with The Novel Materials Discovery (NOMAD) Laboratory, a European Center of Excellence.

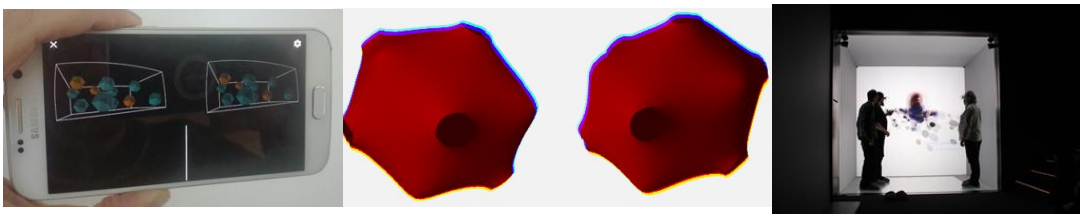

Fig. 1: Crystal structure of Nb_8As_4 (as visualized in Cardboard glasses); Fermi surface of Ag in a Vive system, and adsorption of CO_2 in CaO, as explored in a CAVE system.

[i] CAVE™ is a trademark of the University of Illinois Board of Trustees. We use the term CAVE to denote both the original system at Illinois and the variants developed by multiple organizations.