Virtual-reality view on chemistry and materials science

Rubén Jesús García-Hernández[1], Claudia Draxl[2,3], Matthias Scheffler[3], Dieter Kranzlmüller[1]

1 Leibniz Supercomputing Centre (LRZ), Bavarian Academy of Sciences and Humanities
2 Physics Department, Humboldt-Universität zu Berlin
3 Fritz-Haber-Institut Berlin, Max Plank Society

NOVEL MATERIALS DISCOVERY

Abstract

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 [NOMAD]. The so far implemented functionality covers (Fig. 1) crystal structures, Fermi surfaces, molecular-dynamics trajectories, and electron-hole pairs (excitons). The latter are 6-dimensional objects where virtual reality 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[a] equipment (order Mio. of Euro).

[a] 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.

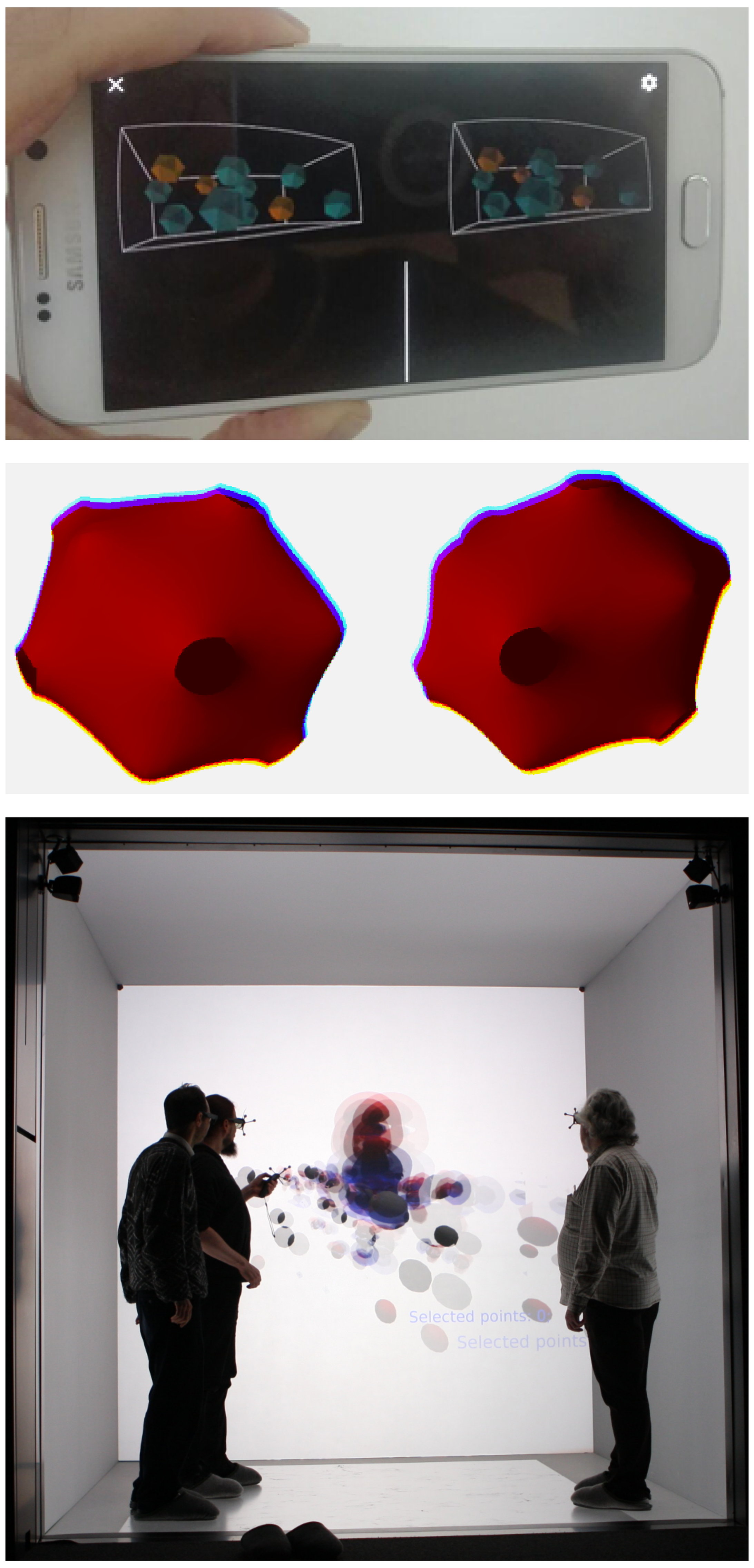

Figure 1: Top: crystal structure of Nb_8As_4 (as visualized in Cardboard glasses). Center: Fermi surface of Ag in a Vive system. Bottom: adsorption of CO2 in CaO, as explored in a CAVE system.

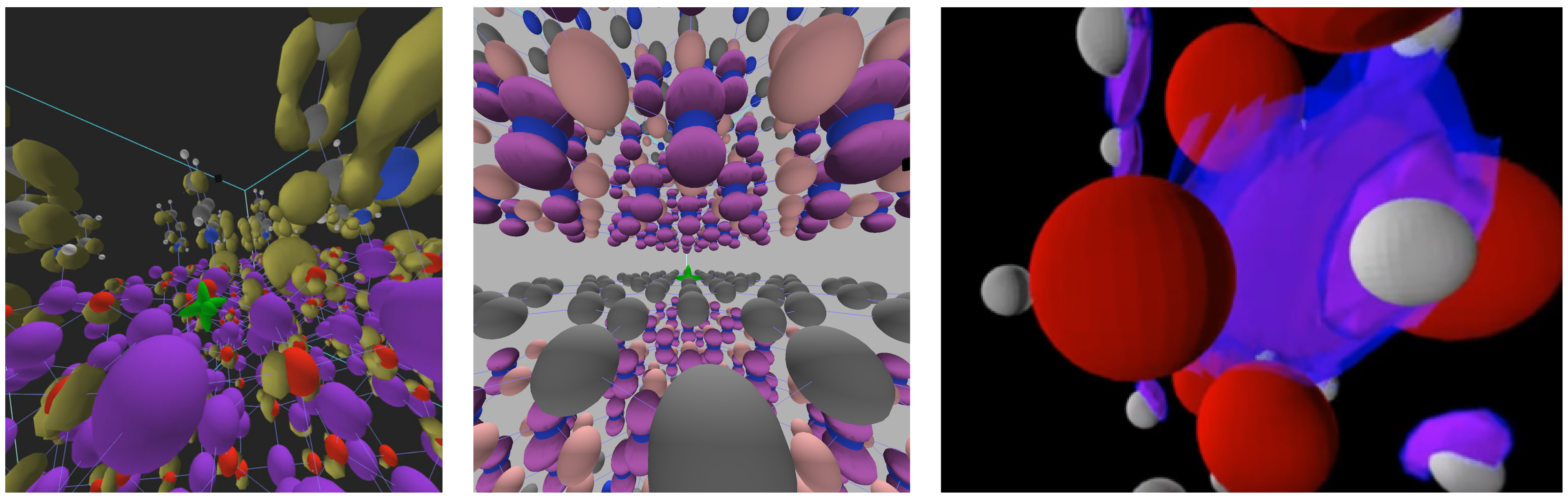

Figure 2: HTC Vive: Excitons for pyridine adsorption on ZnO (left) and graphene-BN heterostructures (center). Stereoscopic, panoramic movie showing excitons in LiF (right).

NOMAD

The Novel Materials Discovery Laboratory, is a European Centre of Excellence (CoE) dedicated to Big-Data in materials science. NOMAD creates, collects, stores, and cleanses data, computed by the most important materials-science codes. NOMAD develops data-mining tools in order to find structure, correlations, and novel information that could not be discovered from studying smaller data sets. The large volume of data and innovative tools will enable researchers in basic science and engineering to advance materials science, identify new physical phenomena, and help industry to improve existing and develop novel products and technologies.

Virtual reality viewer

We have implemented a multi-platform virtual reality viewer [García2017] which can be used to explore and teach different structures commonly used in material science: crystals, Fermi surfaces, molecular-dynamics trajectories, electron density and electron-hole pairs (excitons). Fig. 1 shows examples of the system. We present a demonstration of a 3D visualization of excitons using the HTC Vive. The system allows exploration of the electron density for the different hole positions. We also show 360° stereoscopic movies showing the adsorption of carbon dioxide on calcium oxide and excitons in lithium fluoride. These movies highlight the dissemination and outreach capabilities of immersive visualization techniques.

Excitons

Excitons are hole-electron pairs that are produced when an electron is excited to the conduction band upon absorbing a photon. We visualize an exciton in lithium fluoride (LiF), which is a wide-gap semiconductor with strong electron-hole interaction. The HTC Vive demo shows hybrid excitons in pyridine@ZnO [Turkina2016] and graphene-BN heterostructures [Aggoune2017] (Fig. 2).

Adsorption of carbon dioxide on calcium oxide (CO_2@CaO)

Finding good materials for carbon dioxide capture and activation is useful to reduce global warming and to prepare CO_2 for transformation into more useful chemicals for industry. An example of such materials is calcium oxide. We present a stereoscopic, panoramic video of the adsorption reaction over 423 timesteps (6752 fs). See Fig. 3 for a preview.

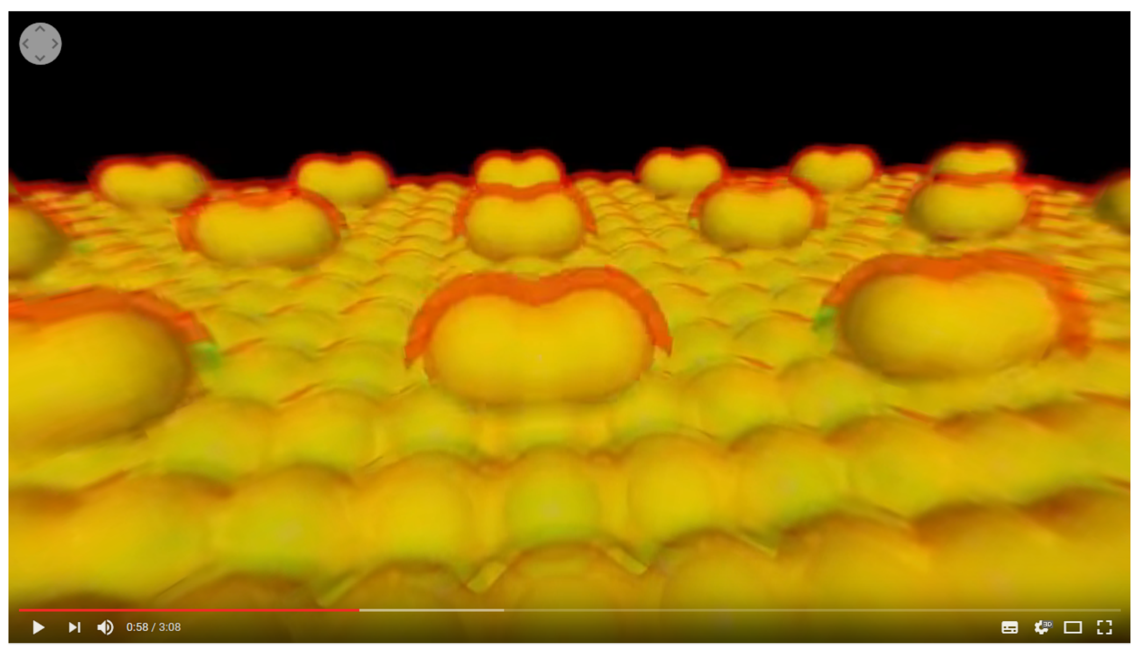

Figure 3: Stereoscopic, panoramic movie showing CO_2@CaO.

Conclusions and future work

Virtual reality tools provide a useful tool to study complex materials. We have shown an effective visualization tool for excitons which can be used for research and outreach purposes. As future work, we plan to implement tighter integration with the NOMAD ecosystem and to make the system more intuitive to use.

Acknowledgements

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. Olga Turkina provided the pyridine@ZnO dataset and Wahib Aggoune provided the graphene-BN heterostructures. The CO_2@CaO dataset was provided by Sergei Levchenko. The Ag Fermi surface was provided by Qiang Fu.

References

[NOMAD] NOMAD Center of Excellence. https://www.nomad-coe.eu/ (2015–2017).

[Aggoune2017] Enhanced Light–Matter Interaction in Graphene/h-BN van der Waals Heterostructures. Wahib Aggoune, Caterina Cocchi, Dmitrii Nabok, Karim Rezouali, Mohamed Akli Belkhir, and Claudia Draxl. J. Phys. Chem. Lett., 2017, 8 (7), pp 1464–1471.

[García2017] Virtual Reality toolset for Material Science: NOMAD VR tools. Rubén Jesús García-Hernández and Dieter Kranzlmüller. 4th International Conference on Augmented Reality, Virtual Reality and Computer Graphics(SALENTO AVR 2017). 12-15 June 2017. Ugento (Lecce), Italy. Lecture Notes on Computer Science, no 10324, Part I, pp 309-319.

[Turkina2016] Electronic and optical excitations at the pyridine@ZnO hybrid interface. Olga Turkina, Dmitrii Nabok, Caterina Cocchi and Claudia Draxl. Computational insight into photo-induced processes at interfaces. CECAM workshop, 10-14 October 2016. Bremen, Germany.