# Virtual Reality toolset for Material Science: NOMAD VR tools

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**Abstract.** We describe a free-software virtual reality system which provides material scientists with a tool to more easily study simulations of chemical systems at the atomic and molecular levels, and which is compatible with the NOMAD infrastructure (an international, open repository which is developing advanced analysis techniques and contains millions of materials). The system runs on multiple virtual reality hardware, from CAVE-like[1] to phone-based. Informal talks with non-domain experts showed positive responses, and a user study was used to confirm the usefulness of the new system by domain experts.

**Keywords:** Portable VR · CAVE · User Study · Material science · CaO · LiF

## 1 Introduction

In this paper we describe a collection of virtual reality tools for analyzing chemical systems in the context of material science. Materials are becoming more complex as user try to optimize for particular properties needed in industrial applications. Supercomputer-based simulations are used to investigate the characteristics of the material and its interaction with other chemicals. In order to effectively visualize the results of the simulations, 3D visualization is becoming a must. In the future, we expect the use of virtual reality techniques to prove invaluable for the study of especially complex materials.

The paper is structured as follows: The next section introduces NOMAD, a framework and database which produces an unified view on materials. Then, some related work in the virtual reality field regarding material science is presented. Section 2 introduces the hardware and SDKs which support our targeted systems. Section 3 describes in some detail two materials which we have used as test cases. Afterwards, section 4 indicates the steps required to transform the datasets commonly used in material science for their use in our virtual reality framework, and provides an overview of the developed software. Finally, section 5

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

details a user study being performed with domain experts and presents preliminary results regarding the advantages of the system with respect to classical software. Section 6 concludes the paper.

### 1.1 NOMAD

The NOMAD repository [14] is an open database of materials (currently hosting more than three million entries), which accepts computer simulations using the most common software packages (called *codes* in the material science parlance).

On top of the repository, the center of excellence [13] is preparing an homogeneus and normalized database. Fourty *codes* are supported, and development continues. An encyclopaedia allowing complex searches regarding the materials stored is being created. Big data analytics will also allow the discovery of descriptors which can be used to find the best material for a given use case lessening the need for expensive computer simulations of million of chemical compounds. Computations-on-demand are also envisioned. Within this project, advanced graphics (both remote visualization and virtual reality environments) will be used to provide better insights into the materials and their properties.

### 1.2 Virtual Reality in Material Science

Virtual Reality provides an immersive virtual world which allows users to enjoy a different reality. 3D glasses and tracking hardware transfer the user to a computer-generated environment, which they can explore and interact with in an intuitive manner. High quality visual and auditive stimuli make the user feel the virtual world as real, commonly also including subconscious responses. The environment can be used for gaming (most commonly), but also for learning, training, research or even for medical treatment of illnesses such as phobias.

In the material science field, Dobrzanski [7] describes a virtual laboratory where users can perform experiments, to be used to practice before using real laboratory equipment, where mistakes can be very expensive. Other similar systems in the experimental chemistry field also exist, e.g. Chemistry Lab VR [16].

In contrast, the work presented here presents the user with the result of three-dimensional simulations of materials at the atomic scale, effectively schrinking the user to the femtometric scale.

There are some virtual reality viewers of chemical reactions, mostly used for educational purposes. For example, alcohol metabolism is explored by Yang et al. [17]. Our work instead provides a general framework for any chemical reaction, and is focused towards research and industry applications.

## 2 Targeted APIs and Systems

See Figure 1 for an overview of the systems targeted. We are supporting the OpenVR[2] and Oculus Mobile[3] SDKs, which while they have been optimized

[2] https://github.com/ValveSoftware/openvr
[3] https://developer.oculus.com/mobile


**Fig. 1.** CAVE-like system (left), HTC Vive (center) and Samsung GearVR (right)

to target specific hardware at the moment (HTC Vive and Samsung GearVR respectively), they are designed to support additional hardware for multiple vendors. OpenVR also supports Oculus Rift.

For the CAVE-like environment at the Leibniz Supercomputing Centre of the Bavarian Academy of Sciences (LRZ), we use an in-house set of libraries which take care of synchronization among the nodes and the projectors.

The system (Figure 1, left) is composed of a cubic, five-wall installation with 2.7m sides. Each side is back-projected using two full-HD stereo projectors which are handled by one rack-mounted PC each. Mirrors are used to reduce the space needed. One extra computer is used for control, tracking and synchronization.

We use tracking hardware from Advanced Realtime Tracking (ART) [4]: a Flystick 3 and tracked stereo glasses. Although only one person can be tracked at a time, we have found collaboration with up to three people is quite confortable, with users looking from behind the tracked users's elbows and obtaining an almost-correct perspective.

In order to have portable tools, we need to ensure that device-independent code can be shared among the different devices. However, due to the lower processing power of mobile devices, we are forced to use a simplified rendering algorithm and to limit the size of the datasets in some cases. The input interface layer must also be tailored for each device.

## 3 Use cases

We have chosen two use cases: a chemical reaction (4D dataset, space + time) and exploration of excitons (6D dataset, 3D electron density for each 3D electron hole position) The 6D dataset is especially interesting for virtual reality, as it is unfeasible for exploration in a normal monitor and it decomposes nicely into two 3D subdomains in virtual reality.

### 3.1 Adsorption of Carbon Dioxide on a Calcium Oxide surface

Carbon dioxide is used in many industrial applications for a variety of purposes. Activation of carbon dioxide is an important step for a further catalytic conversion of $CO_2$ to useful chemicals (e.g., methane) to make renewable fuels. In

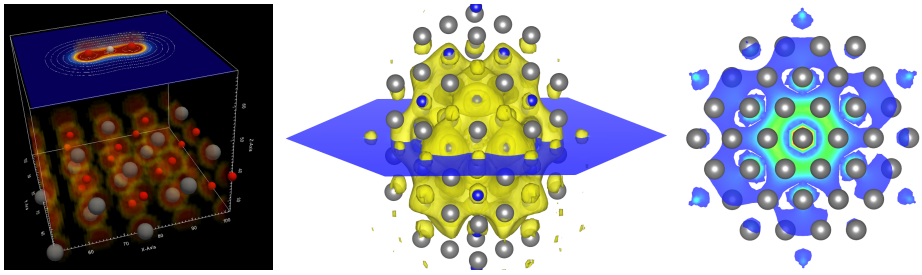

**Fig. 2.** Adsorption of $CO_2$ on CaO(001) surface, using the Paraview software [1] (left), and exciton in LiF, shown in 3D (center) or 2D (right), using the Vesta software [12]

addition, carbon dioxide capture and storage [9] is also one of the techniques proposed to mitigate global warning. Calcium oxide based materials are used for this purpose. Therefore, finding materials which can be used to bind carbon dioxide optimally is of great interest both in the scientific and industry communities.

Our first use case is a molecular dynamics simulation of a molecule of $CO_2$ (3 atoms) on a CaO(001) surface (32 atoms), using a total of 35 atoms for 423 timesteps spanning 6752 femtoseconds (see Figure 2, left). From the simulation, we can learn how electron density and vibrational energy redistribute upon adsorption of $CO_2$ on CaO at a finite temperature. A series of such simulations would allow us to choose a better material for $CO_2$ capture and conversion.

**Interface** In the case of the GearVR, swiping up and down change the timestep, while swiping forward and backwards allows the user to fly in the gaze direction. The back button cycles among the isosurfaces, atoms, and everything.

In the Vive, the triggers allow smooth movement in space and time, while the side buttons move the current isosurface and timestep in discrete steps.

In the CAVE, the joystick allows you to move and rotate the object, while the buttons move you in time. The trigger can be used to cycle the isosurfaces.

### 3.2 Excitons in Lithium Fluoride

Excitons are bound states of an electron and an electron hole, created when a sufficiencly energetic photon interacts with an electron and makes the electron move to a different energy level. They influence the behavior of a material on absorption and emission of light, and are important in opto-electronic applications such as solar cells and lighting devices. Photocathalysis and water splitting are other applications. Excitons in lithium fluoride are a very well studied phenomena [10] so the study of this system with virtual reality tools provides a good baseline to compare against classical tools.

Our second use case is a simulation of the electron density around 344 Lithium and 342 Fluor atoms in a cubic crystal structure, performed for each hole position (see Figure 2, center and right; in 90 % of the cases, researchers are using 2D slices).

**Interface** The hole positions are indicated by a cube of dots located above the controller. One of the dots is marked to indicate the current hole position, and the points are colour coded according to the maximum density at that position. The current hole position can be changed by clicking the controller while pointing it in the direction desired.

The other controller (for the Vive) shows the available isosurfaces. Two buttons can be used to discard non-required isosurfaces and to choose the current isosurface. In the case of the CAVE, the trigger can be used to select whether the isosurface or the hole changes.

## 4 Data Preparation and developed software

In the following sections, we describe the input, processing and output of the pipeline used to prepare the data for our VR software, and the software itself.

### 4.1 Input

We use as input a collection of gaussian cube files [5], which contain a discretized, volumetric representation of electron densities, and a user selection of isovalues.

In the case of the $CaO+CO_2$ reaction, each of the cubes represent one timestep of the reaction. The resolution is 101x101x184 for the full density simulation and 51x51x97 for the relative density simulation. In both cases, 423 timesteps were simulated. Isovalues at 0.85, 2.00, 3.95 and 18.36 were chosen for the demo which was shown to non-expert users, as these can be used to highlight the chemical bond. For domain experts, we used 0.01, 0.05, 0.1, and 0.5 for the full densities and 0.1, 0.05, 0.025, 0.01 (both positive and negative) for the relative densities. These values were requested by a domain expert.

Respectively for the LiF excitons, each of the cubes represent the electron density for a given position of the hole. The resolution is $81^3$ and the hole position was selected from an $11^3$ grid, resulting in 1331 input files. As the electron density depends strongly on the distance between the hole position and the atom positions, we chose isosurfaces as a percentage of maximum densities for this demo. In a first step, isosurfaces from 10% to 80% at 10% intervals were used to find the most interesting hole positions and density levels. Then, after discovering that the region around 20% was to be studied in more detail, isosurfaces from 14% to 26% at 2% intervals were chosen by a domain expert.

### 4.2 Processing

The cube files had to be extended by one unit in each direction to allow the correct extraction of isosurfaces in the case of periodic data, using a python script. Paraview with python scripting was used to export vrml [2] for each isosurface and for the atoms. MeshLab [6] was used to port these vrml files to ply, and for mesh simplification in the case of the first demo. LODs at 50%, 25%, 6% and 2% were used.

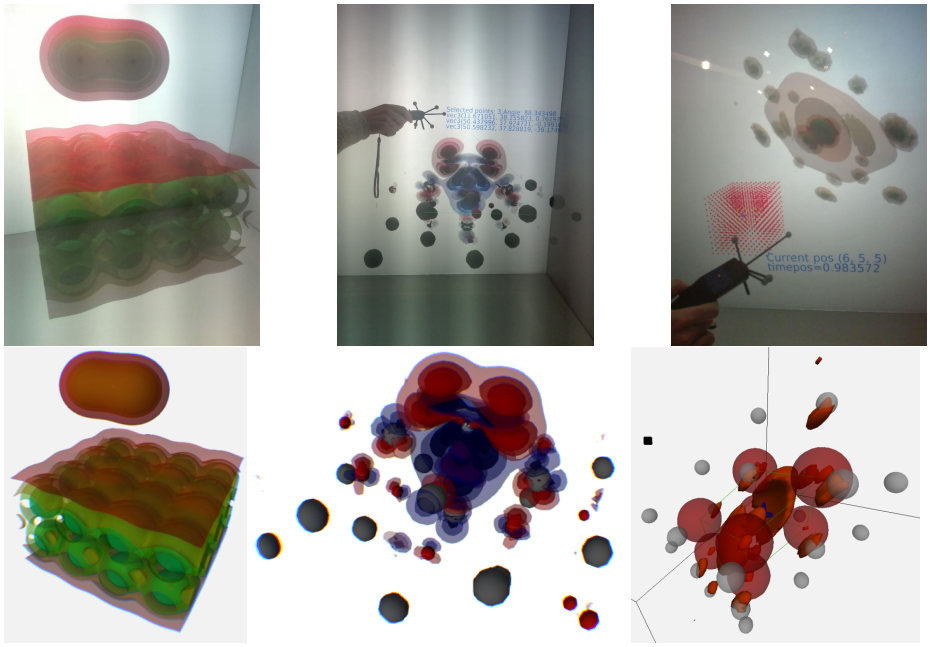


**Fig. 3.** Top: LRZ CAVE-like environment. Bottom: HTC Vive. $CO_2$+CaO(001), full densities (left), relative densities (center). LiF exciton (right)

### 4.3 Developed Software

For the chemical reaction, we have developed a viewer which allows us to move in space and in time, and to show isosurfaces and atoms using isosurface transparency to simulate volumetric rendering. In the case of the GearVR, a low-cost, order-independent additive blending [15] is used. In the other systems, a higher quality depth peeling algorithm [8] is used instead. Isosurfaces and atoms can also be shown as opaque surfaces when needed. Some more details about the adaptations of the interface for the specific usecases can be seen in section 3.

In the case of the GearVR, memory limitations force us to show only half the timesteps for the $CO_2$+CaO full densities demo. In the case of the LiF demo, we have encountered a GCC bug [11] which we are investigating how to mitigate.

Images of the software in action can be seen in Figure 3. The software produced will be distributed as free software under the Apache 2.0 license [3].

## 5 User study and Discussion

We did not try to distinguish which of the supported systems was better. The optimal system depends on the needs and budget of each organization, with the CAVE-like system allowing easy collaboration among multiple researchers (at a much higher cost), while the GearVR can provide a quick overview of

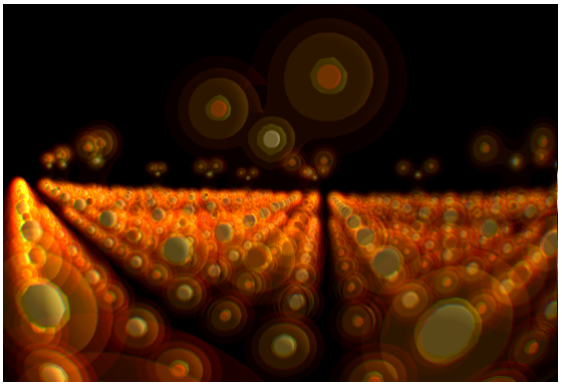

**Fig. 4.** $CO_2$+CaO(001), full densities (left), 7x7 repetitions using LOD simplification

the system at a moderate cost; the Vive system is a compromise solution. We think having a portable system which runs on multiple architectures and having users choose the hardware in accordance with their needs is a more user-friendly approach. Therefore, the purpose of the user study is to compare the systems to the classical, non-immersive PC solutions commonly used in material science.

We have presented an early prototype of the system running on HTC Vive (see Figure 4) to non-domain experts in various public events. The responses were positive, but we did not do a formal user study.

After we prepared demos using isovalues selected by experts on the relevant systems, other experts were shown the systems on the different supported architectures and asked to perform a post-questionnaire using both a 7-point Likert scale and textual answers (questionnaire in Table 1). We distinguish between domain experts and students to assert whether the tool can also be used in teaching and to take into account the fact that domain experts have years of experience using the classic systems, while they very often have not used virtual reality hardware before. We currently are in the process of data collection. Our null hypothesis is that the answer to the questions is 4 (neutral towards the system). The preliminary data analysis of the 15 participants yields a statistically significant advantage (at 95% confidence level, critical value 2,145) of the VR system for questions 1 (4,67±2,23,t=2,32), 3 (5,20±2,41,t=3,85), 4 (5,40±2,37,t=4,58), and 7 (5,00±2,39,t=3,24). We report the 95% interval as $\mu \pm 2\sigma$.

Interaction (questions 2 and 5) and navigation (question 6) at 4,40±2,11,t=1,47, 4,33±2,69,t=0,96, and 4,27±3,34,t=0,62, respectively, are only found to be slightly easier in the VR system, and the results for these questions are not significant. More work needs to be done to provide an easier-to-use system. Question 8 (4,20±2,64,t=0,59) indicates a non-significative, slight preference for VR use.

A general view was used by averaging the answers to questions 1-8. The result is 4,683±1,997, t=2,65: slight, but significant, preference for the VR system.

Users provided in questions 9-14 valuable input about their views on the advantages, disadvantages and application areas of the system. In general, the

**Table 1.** Post-Questionnaire

1. I find navigating the VR system easier
2. I find interacting with the VR system easier
3. I find understanding the visualization in the VR system easier
4. I think students will have an easier time understanding concepts by the use of the VR system
5. I think students will find navigating the VR system easier
6. I think students will find interacting with the VR system easier
7. I think students will find understanding the visualization in the VR system easier
8. I prefer the VR system to systems I have used previously for similar tasks
9. In general, do you think the use of VR in this specific example is positive or negative?
10. Can you foresee having an easier time discovering new phenomena by using VR systems like this?
11. Can you think of any study which can be performed more easily on the VR than in classic systems?
12. Can you think of any study which can be performed more easily on the classic systems?
13. Can you think of any additional benefits of the VR representation?
14. Can you think of any additional drawbacks of the VR representation?

answers to question 9 were positive towards the VR system, while 10 had 6 positive and 3 negative answers. The many possible studies mentioned in question 11 and 12 show that both VR and classical software systems will coexist with each providing advantages in different scenarios. Textual comments by users follow:

With respect to new discoveries using VR (question 10), VR can provide new insight for the following reason: Manual inspection of large datasets is impossible, i.e. the person who has carried out the calculation would need to screen every electron/hole combination to get the full picture. While this is still possible for simple systems like LiF, it is not feasible for complex materials. Also, with the VR tools in hand, this knowledge is accessible to a larger community.

The following studies were presumed to be performed more easily in VR (question 11): Cosmology/star formation studies, 4D systems like time evolution, space-time systems, trajectories, dynamical phenomena, chemical reactions, Complicated systems with a lot of detail, and some tasks within certain studies.

On the contrary, some studies are perceived to be easier to perform on classical systems (question 12): 3D excitons, Rayleigh-Jeans instability, where you usually represent your results with a single slice through the volume, 2D visualizations allow for plots that are more easily analyzed at the PC and presented in talks or publications, 3D visualizations without VR, which allows for projections along different crystal axes (giving insights into the symmetry of the wavefunction). In the case of simple systems, non-VR is also preferred.

The advantages of the system (question 13) are: providing a better representation and understanding of the spatial extension/distribution of phenomena,

more complete understanding of the problem, allowing the user to directly interact with the representation, powerful visualization tools for specific excitations where the real-space character is of particular interest, such as charge-transfer excitions (helping understand the influence of the wavefunction on both hole and electron position), and scanning for interesting configurations could be easier. In particular, rotating a complex 3D system using the traditional 2D display is hard, and there is potential to become easier than an equivalent 2D system. It is much easier to focus on certain parts of a complicated system. It is also an attractive educational instrument for young students, and allows broader outreach to the non-scientific audience.

With respect to drawbacks (question 14): there is a possibility of over-interpretation of the visual data, as the interpretation of the 6D wavefunction is –in principle– highly non-trivial and its determination requires a careful calculation with extensive tests and convergence checks. Multiple users mentioned the need for extra hardware, the lack of availability of VR infrastructure, its cost and difficulty of setup, or logistics problems. The technology is under development and specialized, and often single-user. Some users found it cumbersome, harder to navigate, tiring for daily work, or requiring too much effort compared to the benefits for the specific example. In particular, the system is very sensitive to the quality of the loaded data, and the data volume is high.

## 6 Conclusions and future work

We have developed a virtual reality viewer for material science simulations and compared it to the classical software used in the field. Although the system is still an early prototype, domain experts consider that it can be useful in a variety of tasks and think that it is a valuable addition to their tools; however, the state of the technology is still seen as experimental, unavailable, costly or difficult to setup by end users. A small, albeit statistically significant, advantage of the VR system with respect to traditional tools is confirmed by the user study. More work needs to be done, though, to easen interaction and navigation in the virtual world and to add more functionality to the system.

For future work, we would like to use real-time volume rendering to provide higher-quality visuals and to avoid the pre-selection of isosurfaces. We would also like to investigate ways to present the exciton datasets in the GearVR, and to increase the functionality of the demos. We must also work on generalizing the demos to work in other types of datasets and to integrate them with the NOMAD encyclopaedia. Additional functionality from the classical tools used in material science should be ported to the VR system as well, under guidance from domain experts. Finally, we would like to also target other VR devices.

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