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Entering the Augmented Era: Immersive and Interactive Virtual Reality for Battery Education and Research**

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We present a series of innovative serious games we develop since four years using Virtual Reality (VR) technology to teach battery concepts at the University (from undergraduate to doctorate levels) and also to the general public in the context of science festivals and other events. These serious games allow interacting with battery materials, electrodes and cells in an immersive way. They allow experiencing impossible situations in real life, such as building with hands battery active material crystal structures at the nanometer scale, flying inside battery composite electrodes to calculate their geometrical tortuosities at the micrometer scale, experiencing the electrochemical behavior of different battery types by driving an electric vehicle and interacting with a virtual smart electrical grid impacted by 3D-printed devices operated from the real world. Such serious games embed mathematical models with different levels of complexity representing the physical processes at different scales. We describe the technical characteristics of our VR serious games and their teaching goals, and we provide some discussion about their impact on the motivation, engagement and learning following four years of experimentation with them. Finally, we discuss why our VR serious games have also the potential to pave the way towards an augmented era in the battery field by supporting the R&D activities carried out by scientists and engineers.

1. Energy Storage and Virtual Reality

Energy storage is one of the most prominent challenges Humanity has to face in the 21st century.[1] This is mainly due to the increasing use of smart grids and of variable renewable energies driven by the limitation of fossil fuels and the climate change.[2] Electrochemical energy storage technologies such as lithium-based rechargeable batteries are called to play a major role to address this challenge, due to the simplicity of their overall operation principles and high energy densities. Since their first commercialization in 1991 by Sony, lithium-ion batteries (LIBs) have triggered the emergence of a wide spectrum of portable devices and they are nowadays enabling the renaissance of the electric vehicles (EVs).[3–5] The desired massive electrification of the transportation sector still requires better rechargeable battery technologies than current LIBs in terms of specific energy, cost, recyclability, and safety. To make this happen, the design of advanced LIBs with a new generation of electrode materials and smart functionalities (*e.g.*, embedded state of health sensors and self-healing actuators) is required.[6] Other lithium-based rechargeable battery technologies have emerged at the laboratory scale and have been the focus of intense studies in the last decades such as lithium–sulfur batteries (LSBs) and lithium–oxygen batteries (LOBs) due to their higher theoretical specific energies than the ones achievable in current LIBs.[7,8] However, significant technical challenges still persist in LSBs and LOBs, such as the premature capacity fading in the former and the severe instability of the electrolyte and poor rechargeability in the latter.[9,10]

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In general, any scientific approach adopted to try to overcome the aforementioned technical challenges as well as to design and optimize any kind of electrochemical energy storage device, requires transdisciplinary efforts, encompassing at least materials science, chemistry, physics and engineering. Indeed, lithium-based batteries are made of multiple materials and their operation implicate numerous physicochemical mechanisms occurring simultaneously at multiple spatial scales.[11] To successfully implement the required transdisciplinary approaches and to favor the invention of disruptive energy storage technologies, it is of paramount importance to encourage the emergence of tools that can ease the inspiration by the current and the future generations of battery scientists. Virtual Reality (VR) technology constitutes one of such tools because it can ease training, education, and stimulate creativity in research.

VR environments were adopted very early for training in abstract or complex situations.[12] They have been revealed very useful for training in the cases when the possibility to perform *in vivo* situation is either difficult, expensive or dangerous (*e.g.*, in spatial, military and nuclear areas).[13–17] The immersive experience in an environment inspired by physically realistic phenomena in which it is possible to interact represents an important asset of VR: this helps users at developing an intuitive knowledge about the simulated system.[18] Thanks to the recent technical progresses, VR hardware has become more compact and accessible to much wider audiences: Oculus and HTC Vive are examples of commercial VR hardware.[19–20] These technologies have head-mounted displays that allow easy interaction with the virtual environment by using controllers equipped with motion tracking (Figure 1).

In the recent years, VR technology started to be significantly used for educational and research purposes in hard sciences such as mathematics, physics and chemistry.[21–25] In chemistry, especially, researchers have proposed VR tools to visualize quantum mechanics and molecular dynamics simulation results or to teach experiments in immersive and interactive way.[26–32]

In the battery field, we can think that VR has also strong potential to provide a fully immersive and interactive experience that can tremendously ease the understanding of concepts behind materials, components, cell and packs working principles. VR could be used to put the users in situations that are impossible in reality, such as manipulating and navigating inside a material of few micrometer size by interacting and by measuring the consequences of the interactions in real time. Surprisingly, despite these tremendous promises, the use of VR in the battery field has never been reported. Instead, the most used traditional way providing virtual experience in the battery field is computational modeling. Since more than 50 years computational models have revealed to be useful *simulation* tools to understand battery operation principles and to carry out their design and optimization.[11,33] Such models are based on mathematical equations describing physicochemical mechanisms which are solved by using informatics programs. Therefore, the models constitute virtual materials or batteries with which one can perform virtual experiments, such as investigating how operation conditions (*e.g.*, applied current density) impact outcomes such as the capacity or the aging. Numerous models have been proposed under several geometric representations of the cells and the electrodes within, in one dimension (1D), two dimensions (2D) or three dimensions (3D).[11] However, the efficient development and use of these models require some programming skills. Moreover, the visualization of results arising from 3D models (*e.g.*, spatial distribution of chemical species in the electrodes) is not trivial: images remain "confined" in 2D computer screens. This issue of 2D representation of 3D objects make that often students and battery researchers are confronted to difficulties in the abstraction and conceptualization in three dimensions of battery materials and components, such as the active material crystal structures at the nanoscale, the composite electrode porosity at the mesoscale and the theoretical operation principles of these batteries in real applications. Some educators and science communicators have used classical 3D glasses (like the ones to watch movies in theaters),[34] but these glasses do not permit individual or collective interaction with the objects and immersion into them.

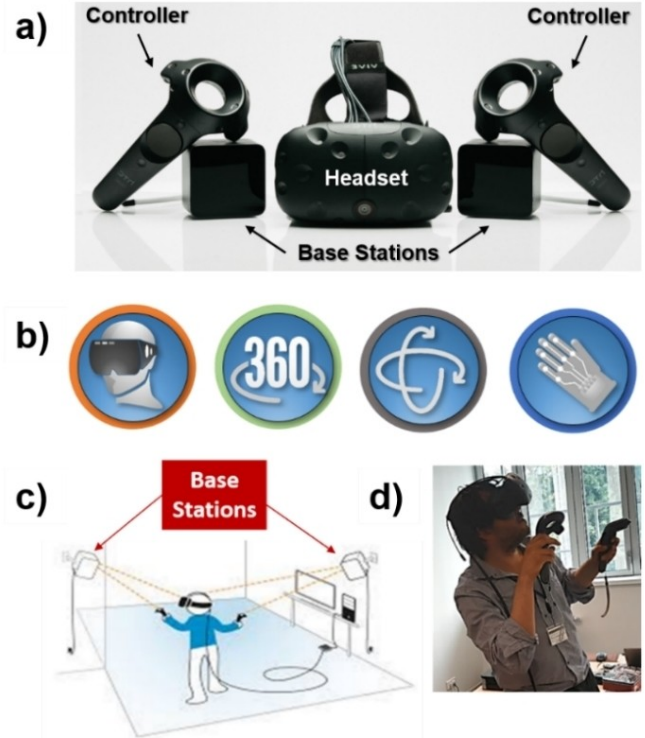


Figure 1. a) Illustration of the HTC Vive VR hardware (adapted from Ref. [20]); b) overall principles (need of a head-mounted display, virtual environment in 360°, full immersion, full interaction using controllers); c) typical location of the base stations and the user (adapted from Ref. [20]); d) a VR user in action.

In this Concept, we report six VR *serious games* we started to develop four years ago, allowing students and researchers to interact in an immersive and realistic way with virtual battery materials, composite electrodes, battery cells in EVs and smart electrical grids, as well as with the mathematical models used in the VR environment simulations. With serious games[35–36] we refer here to games designed for learning the operation principles of rechargeable batteries, with the aim at rising the motivation, the engagement and the learning efficiency by students and by the general public, and also to stimulate the creativity of battery researchers. Our pedagogy activities using these VR serious games were recently recognized with one of the French National Prizes for Pedagogy Innovation in 2019 (PEPS 2019).[37–40] The goal of this Concept is to present the main characteristics and pedagogical goals of these VR serious games, as well as some illustrations of their utilization in the last four years. Some discussion about the impact on the motivation and learning by students and other users in general is also provided, without the intention to share here detailed ergonomic and psychological assessments in view of the readership of this Journal. Such assessments are being shared by us elsewhere (see for instance Ref. [41]). We also discuss the potentialities of these VR tools to boost battery R&D.

2. Battery Virtual Reality Serious Games

All our VR serious games were coded using Unity programming language and Revia® technology.[42] Some of them contain Python scripts allowing the modification of some of their features (see below) via user-friendly interfaces. Our serious games were developed to operate with HTC Vive hardware connected to a PC or laptop powered with a graphical card with Nvidia GTX1060 as minimal required configuration. The HTC Vive system allows for robust room-scale tracking, permitting the user to move around naturally. However, the games could be ported to other systems, such as Oculus Rift, with minimal changes.

2.1. Crystal VR Serious Game

In a charged LIB cell, lithium is hosted in the active material of the negative composite electrode also made of carbon additives and binder. Upon discharge, lithium de-intercalates from the active material and migrates through the electrolyte filling the pores of the composite negative electrode and the separator, towards the active material present in the composite positive electrode where it intercalates (Figure 2). The macroscopic voltage response of these batteries is therefore a complex function dependent on numerous factors, such as the chemical and structural properties of the active material crystals used in the electrodes, the mesostructure of the electrodes, the electrolyte composition and the cell operation conditions (*e.g.*, applied current density).

The *Crystal VR* serious game, developed by us in 2019, addresses the structural (crystallographic) properties of the active materials.[43] Teaching crystallography to students often faces a dilemma. How to draw in two dimensions symmetry operations and crystal structures which are by nature three-dimensional? Of course, perspective drawings are used, but still, some students and even battery researchers are not at all able to clearly see (and thus to understand) a 3D representation on a 2D plan.

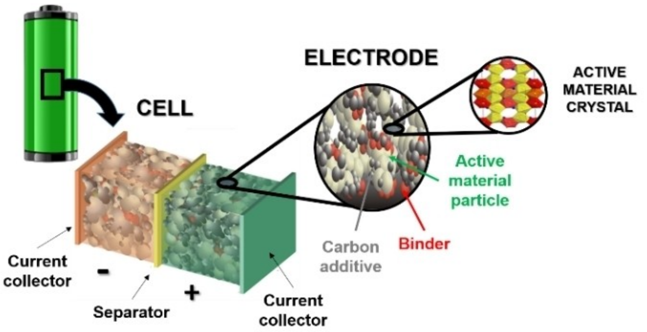


Figure 2. Multiscale character of a LIB cell. The active material crystals constitute the smallest operational component of the composite electrodes.

The crystal structure of any material is the periodic repeatability of a so-called "unit cell" in the three directions of space. This "unit cell" is constituted of atoms (same or different chemical nature) related by symmetry operations. If we remove the elements of symmetry, we obtain what is called the "asymmetric unit". Taking the example of table salt (NaCl), we can see that the "asymmetric unit" is made from only two atoms (one sodium atom and one chlorine atom depicted as yellow and green spheres respectively in Figure 3). However, adding symmetry operations, it turns out that the chlorine is actually surrounded by six sodium atoms in a very specific arrangement called octahedron in the "unit cell". Finally, all those "unit cells" are repeated in the three directions of space, forming *in fine* the salt crystal.

In crystallography, symmetry operations are divided into four main categories:

- Mirrors (labelled "*m*");
- Rotations axis of different orders *n* (rotation of $2\pi/n$ with $n=2, 3, 4, 6$);
- Glide planes (mirror + translation labelled *a*, *b*, *c*, *n*);
- Screw axis (rotation of order *n* + translation labelled 2_1, 3_1, 3_2, 4_1, 4_2, 4_3, 6_1, 6_2, 6_3, 6_4, 6_5).

As mentioned earlier, explaining and visualizing the symmetry operations is not an easy task. As it can be seen on Figure 4, being able to differentiate a mirror and a rotation axis of order 2 ($2\pi/2=180°$) is not trivial, especially when using spheres (which are highly symmetrical objects).

Using VR reveals to be of great interest for students in order to understand those notions of symmetry and crystal structure representation. Our Crystal VR serious game gives access to the

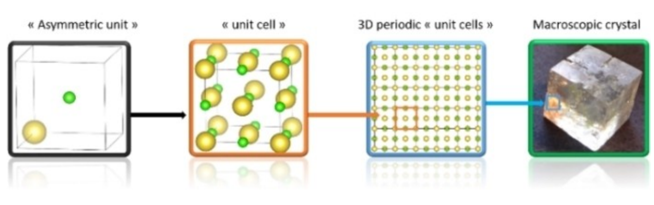


Figure 3. Constitution of the table salt (NaCl) from the macroscopic crystal down to the "asymmetric unit".

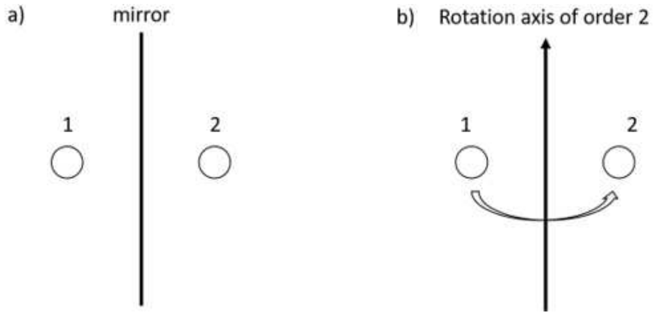


Figure 4. Effect of a) a mirror, and b) a rotation axis of order 2. The initial sphere is labelled "1" and "2" after applying the different symmetry operations.

user to a virtual room proposing two virtual workshops dedicated to the visualization of different symmetry operations and the construction of crystal structures (Figure 5).

2.1.1. Symmetry Operation Workshop

This workshop (Figure 5a) aims to help students to visualize a set of symmetry operations. The student should first select an element of symmetry from a set of operation such as a mirror, rotation axis (order 2 and 3), screw axis 2_1, etc. The element of symmetry can be freely placed in the 3D space using the VR controller. In order to see the effect of the chosen symmetry operation, the students must then select a daily-life object (a car with a driver, a guitar, a pan, a Lego® Man, Chinese Lucky Cat, etc.). The selected object can also be freely positioned aside to the element of symmetry and the image generated through this symmetry is automatically created. The aim of choosing such objects is two-fold: i) those objects do not have a high degree of symmetry which allows to better see the effect of the different symmetry operations compared to spheres and ii) it makes the serious game more "playful" and thus more attractive to the students.

2.1.2. Crystal Structure Workshop

After becoming more familiar with the different symmetry operations used in the first workshop, students can use this knowledge to understand how a complete crystal structure (all atoms in the unit cell) is built from the asymmetric unit using different symmetry operations (Figure 5b). To do so, several typical crystal structures are available. For instance, the crystal structure of table salt NaCl can be selected. The complete crystal structure (all atoms in the unit cell) is thus displayed and it is then possible to interact with it using the RV controllers. First, it is of course possible to zoom in and out. This means that it is either possible to "walk" into the crystal and see under different angles how the atoms are arranged or hold it in your hand (Figure 6). Second, still using the controllers, it is possible to move the atoms away from their original position and see in real time how this will affect the crystal structure. Another feature allows to change the chemical nature of the different atoms and also to build its own crystal structure from an empty unit cell.

Both *Crystal* workshops are very versatile so that changes and improvement can be easily made. The *Crystal Structure* workshop has been developed as a tool to better visualize crystal structures. We can imagine creating exercises in which students are asked to construct specific crystal structure types.

Figure 6. A player using Crystal VR serious game.

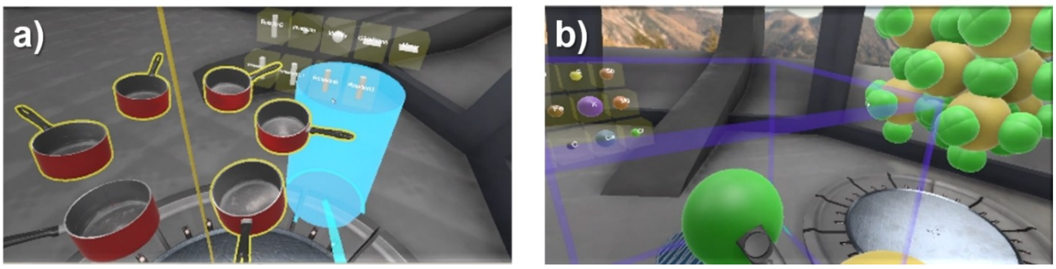


Figure 5. Screenshots of the Crystal VR serious game; a) Symmetry Operation workshop; b) Crystal Structure workshop. Video provided in the Supporting Information.

They should select the proper unit cell, the proper atoms and element of symmetry in order to build the proper crystal structure. Another improvement could be the display of the X-ray diffraction pattern created from the selected (or created crystal structure). X-ray diffraction is used every day in laboratories working in the battery field. An X-ray source illuminates a sample, which reflects (diffracts) the X-ray beam. We obtain the so-called X-ray diffraction pattern consisting of a succession of peaks with different intensities, from which crystallographers can deduce the crystal structure of a given material. The position of the peaks are related to the size of the "unit cell" described above and their intensities to the chemical nature and the position of the atoms into the "unit cell". But, it is also possible, knowing the exact crystal structure, to predict and calculate what the X-ray diffraction pattern should look like. It will be indeed very interesting for students to be able to see such simulated patterns corresponding to the crystal structure they are looking at and observe how the pattern evolves when they change the chemical nature of the atoms, their positions and so on. Furthermore, battery researchers are really interested in being able to "fly" into crystals. It is possible to imagine an evolution of *Crystal VR* to see and follow the diffusion path that a Lithium or a Sodium ion is taking when migrating through the active material. This could allow researchers to better understand why a given electrode material is more efficient than another one and consequently, could help them to design new materials with enhanced properties.

2.2. Tortuosity VR Serious Game

LIB composite electrodes are made of a complex mixture of active material, carbon additive and binder, forming a three-dimensional porous mesostructure which needs to be filled with electrolyte in order to ensure the proper exchange of lithium ions between the two electrodes constituting the cell (Figures 2 and 7a). Both the porosity and the average geometrical tortuosity of the electrode are recognized to play a crucial role at determining the overall transport properties of lithium ions in the electrolyte, and therefore the practical characteristics of the LIB cell such as its power density.[44,45] The *Tortuosity VR* serious game, developed by us in 2018, addresses the geometrical tortuosity of battery electrodes.

The geometrical tortuosity [Equation (1)] is defined as the ratio between the travelled distance between two points (L_{AB}) (Figure 7) at two opposed borders of the electrode and the thickness of the electrode along the motion direction ($L_{electrode}$):

$$\tau = \frac{L_{AB}}{L_{electrode}} \tag{1}$$

The effective diffusion coefficient of the lithium ions in the electrolyte is given by Equation (2):[46]

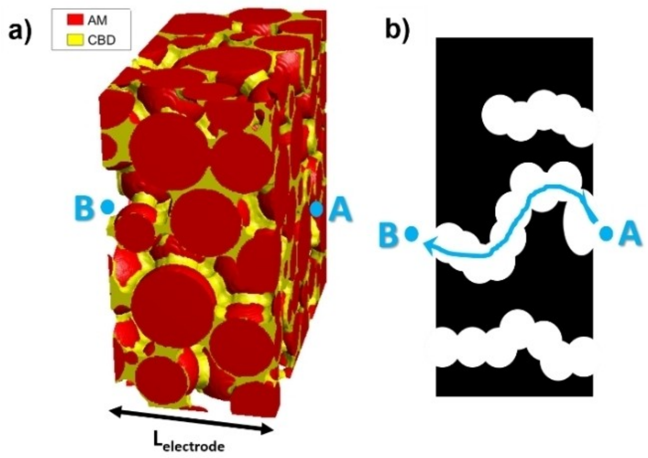


Figure 7. a) Schematics of a LIB composite electrode, illustrating the active material (AM) and the carbon binder domain (CBD). Points "A" and "B" used in the definition of the geometrical tortuosity [Equation (1)] are also indicated. $L_{electrode}$ stands for the electrode thickness; b) traditional (bi-dimensional) way of illustrating the concept of "tortuous path" (arrow between points A and B). Note that the porous channel on the top has infinity geometrical tortuosity whereas the one at the bottom has lower geometrical tortuosity than the one in the middle.

$$D_{eff} = \frac{\varepsilon}{\tau^2} D_{bulk} \tag{2}$$

where the porosity ε is defined as the ratio between the volume occupied with electrolyte in the electrode and the volume of the electrode.

Even if the geometrical tortuosity concept is easy to understand in two dimensions (Figure 7b), its understanding in three dimensions is not trivial at all as it requires imagining three-dimensional paths for no discontinuous transport between one side and the other one of the electrodes. Numerous students and battery researchers have difficulties at imagining and visualizing such three-dimensional paths. This is why numerous theories exist aiming at calculating the geometrical tortuosity of electrodes as function of their porosity, the most famous one being the Bruggeman relation [Equation (3)] postulating that:[47]

$$\tau = \frac{1}{\sqrt{\varepsilon}} \tag{3}$$

However, these theories assume the electrodes to have unrealistic ideal geometries. In the case of the Bruggeman relation above, it holds when the electrode is constituted by spherical particles and with low volume fraction. It has been demonstrated that other particle shapes lead to other mathematical expressions relating the geometrical tortuosity to the porosity.[48] Transmission line models have been used to assess the geometrical tortuosities of LIB electrodes from the fitting of their parameters to Electrochemical Impedance Spectra.[49] However, electrodes are tri-dimensional objects and therefore they have three geometrical tortuosity values, along the cartesian directions X, Y and Z. Very different values of

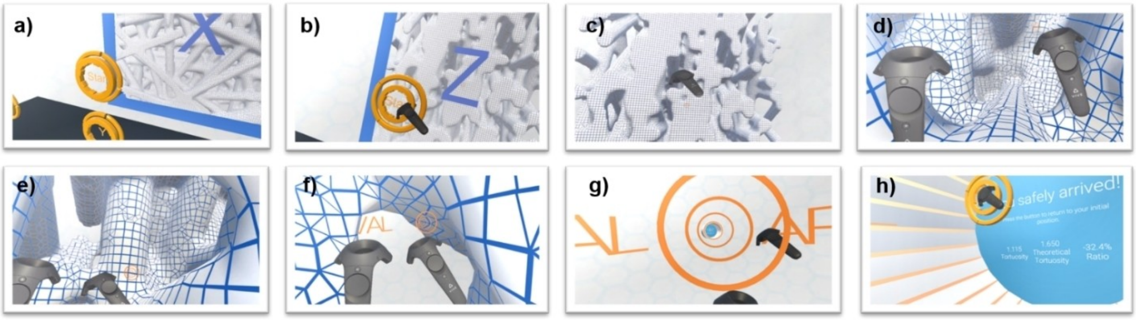


Figure 8. Snapshots of the *Tortuosity VR* serious game along different utilization instants, from the selection of the flight direction (a,b), to the flight itself (c,d, e,f) and the arrival to the cylinder showing the calculated and the theoretical geometrical tortuosities values (g,h). Corresponding video provided in the Supporting Information.

these three tortuosities would mean a highly anisotropic electrode. Such anisotropy can lead to heterogeneities of the battery operation.[45] Evaluating such tortuosity anisotropy is of major importance. Commercial software such as GeoDict[50] and applications like TauFactor[51] allow evaluating such geometrical tortuosity values by solving steady state Fick's laws. However, these numbers are averaged. We believed that designing a tool that can transform a student or a researcher in a "ion" moving in the electrolyte filling the pores can be really interesting to apprehend the path-dependence and the anisotropic character of the geometrical tortuosity and better analyze its impact on the overall electrode operation principles.

The *Tortousity VR* serious game proposes to the user to fly along the thickness of electrode mesostructures in order to calculate their geometrical tortuosities (Figure 8). The user can choose among X, Y and Z directions by holding one of the HTC Vive controllers. At the beginning the user is facing the side "X" of the electrode. When the controller is placed on "Y" or "Z" circles, the electrode turns to face its "Y" or "Z" sides to the user. When ready, in order to start to fly, the user places the controller on "start". Once flying, when the user extends his/her arms he/she accelerates, while when bringing back the arms to his/her chest the user slows down. If the user touches the solid material constituting the electrode she/he will be back to the starting point with the possibility of choosing the same direction or another one to fly along. In order to find his/her way (in case of finding an impasse), the user has also the right to fly back (towards the starting point) but no longer than 10 seconds.

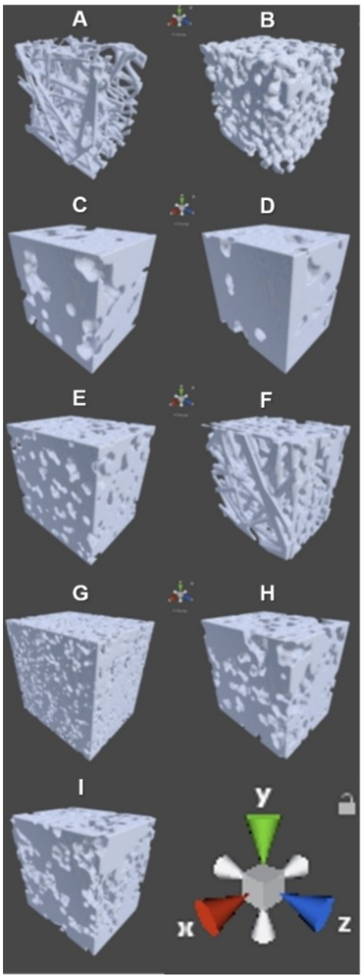
If the user is successful at going across the electrode along the chosen direction, she/he will meet an arrival cylindrical spot. Such cylindrical spot is visible from inside the electrode and helps at orientating the player to escape from the electrode. By entering in the cylindrical spot, the player discovers the ratio between the theoretical geometrical tortuosity value (calculated using the GeoDict software) and the value calculated from the flight distance L_{flight} following

$$\tau = \frac{L_{flight}}{L_{electrode}} \tag{4}$$

The Tortuosity VR serious game has been used with ten different electrode mesostructures (cubes of $50\times50\times50\ \mu m^3$, magnified approximately 20000 : 1), generated by using GeoDict software, each of them having different theoretical geometrical tortuosities also according to the adopted direction. Nine of the used electrode mesostructures and the corresponding theoretical values of geometrical tortuosities are reported in Figure 9. It can be noticed that for one particular electrode mesostructure the geometrical tortuosity is infinity along the Y direction: that means that it is impossible for the player to find a way to arrive to the other side of the electrode. Except for that case, and depending on the speed of flight and the complexity of the electrode mesostructure, typical duration of a successful game (*i.e.*, where the player successfully goes across the electrode mesostructure and arrives to the arrival cylinder) is comprised between *ca.* 1 and 5 minutes. The game records the accomplished path by the last successful player: this can be used as a guideline by the next player.

This serious game allows learning about the anisotropic character that the geometrical tortuosity has in battery electrodes (Figure 10). Such anisotropic character depends on their manufacturing process. It also allows learning that the geometrical tortuosity is a path-dependent property (cf. Figure 7b legend). Besides its strong educative interest, *Tortuosity VR* reveals to be a very useful tool in R&D to analyze in more deep battery electrode mesostructures and to calculate their geometrical tortuosities without having any programming skills: tortuosities calculations become literally a child's play.

The serious game is flexible and can also support other types of electrode mesostructures obtained by computer tomography or by simulations of the electrodes manufacturing process. In an evolution of the game, we plan to highlight the spatial location of the carbon binder domains (CBDs) in the LIB electrode mesostructures to allow the player to quantify while flying the "death zones" of the active material towards lithium (de-)intercalation. The game can also be applied to electrodes in other types of batteries or electrochemical devices. It can be also easily extended to fly through other components such as separators or any other kind of porous media, or crystal structures representing active materials or solid electrolytes.



	A	B
X	1,08	1,34
Y	1,09	1,33
Z	1,10	1,34

	C	D
X	2,21	4,11
Y	1,90	Infinity
Z	2,78	5,56

	E	F
X	2,75	1,32
Y	2,95	1,32
Z	2,74	1,65

	G	H
X	2,2	2,75
Y	2,2	2,86
Z	2,18	2,68

	I
X	1,87
Y	2,08
Z	1,77

Figure 9. Different electrode mesostructures available in the *Tortuosity VR* serious game, with the theoretical values of geometrical tortuosities along the cartesian directions.

2.3. Nanoviewer VR Serious Game

Nanoviewer VR serious game was developed by us in 2017 to allow a user to manipulate in an immersive environment a wide diversity of digitalized battery-related objects such as electrolyte molecules, active material or solid electrolyte crystals and composite electrode mesostructures (Figure 11). The goal here is to ease their visualization and assessment of asymmetries, anisotropies, and spatial organization of the materials in three dimensions. *Nanoviewer VR* is the precursor of *Crystal VR* and *Tortuosity VR*, but it allows manipulating any kind of digital object without other purpose than the visualization. Molecules and crystals can be originated from any kind of software for atomistic and molecular analysis and calculations, such as LAMMPS[52] or VESTA,[53] provided that the output files from these software are recorded in an atom-type file format. The composite electrode mesostructures can be originated from tomography characterizations or by using a physical model simulating their manufacturing process. The latter model, already reported by us,[54–57] is supported on a Coarse Grained Molecular Dynamics (CGMD) approach simulating LIB electrode slurries and the resulting electrode mesostructures upon the slurry solvent evaporation. By using CGMD, we have calculated several electrode mesostructures resulting from several formulations quantified by the weight ratio between $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ active material particles and carbon-binder, and the $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ particles size distribution.[54–56] Figure 11 shows the example of a LIB composite positive electrode of $50\times50\times50\ \mu m^3$ of volume, where large particles represent the $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ active material and small particles represent the CBDs. The latter contain PVdF binder and carbon nanoparticles, merged as single domains. CBDs have the role of ensuring good electronic

Figure 10. A student playing with our *Tortuosity VR* serious game. What is seen by the student in the VR environment is simultaneously projected in a traditional screen to allow others to see as well (Photo taken by Cyril Fresillon, Photothèque CNRS/LRCS, Copyright CNRS. Reproduced with permission).

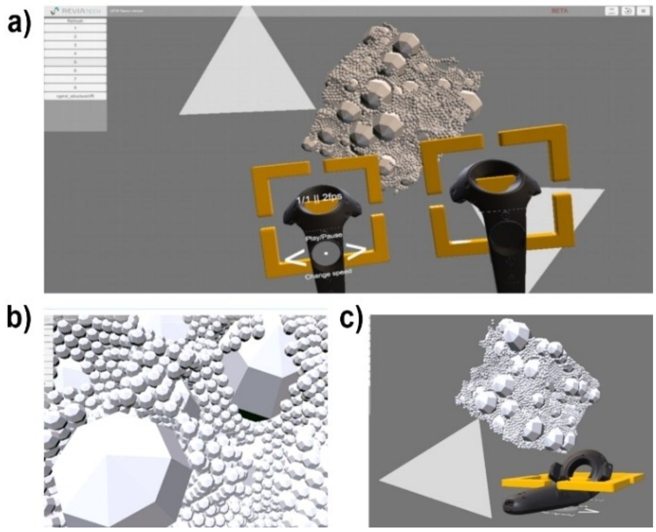


Figure 11. a) Snapshot of the *Nanoviewer VR* serious game when manipulating an electrode; b) zoom; c) rotation. The electrode in this example has a mass composition of 90% active material and 10% of carbon-binder particles. The volume of the electrode visualized in the VR environment is of 50 x 50 x 50 μm^3. Corresponding video provided in Supporting Information.

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percolation between the composite electrode and good adherence between the active material particles.

Several types of interactions are possible with the digital objects and the composite electrode mesostructures, in *Nanoviewer VR* (Figures 11 and 12):

- enlarge the digital object, using a movement of arm spacing, with both handles, to be able to "dive" inside the materials, composite electrodes, etc.;
- shrink the material or composite electrode mesostructure, using a movement of arm spacing, always with both handles;
- using a single handle, grab the material or electrode mesostructure to rotate it, move it in space, move it away or move it closer together.

Nanoviewer VR was used to perform several types of activities with students such as discovering how active materials and CBDs are organized in three-dimensions in composite LIB electrodes, evaluating the porosity of the electrodes and the surface area of contact between active material particles and CBD, and search for hidden objects ("easter eggs" like cubes and other polyhedra) in a limited time (60 seconds) (Figure 13). The spatial organization of these materials in a composite electrode determine its practical properties: for instance, the surface area of contact between pores and active material determine the power density of the composite electrode. Indeed, as parts of active material covered by CBD will remain electrochemically less active towards Li insertion or de-insertion, despite CBD may contain some microporosity, the path for Li^+ to move through can be significantly tortuous.[56,58] Other practical properties of LIBs will be affected by such interfaces, such as the cell durability and the safety.[59]

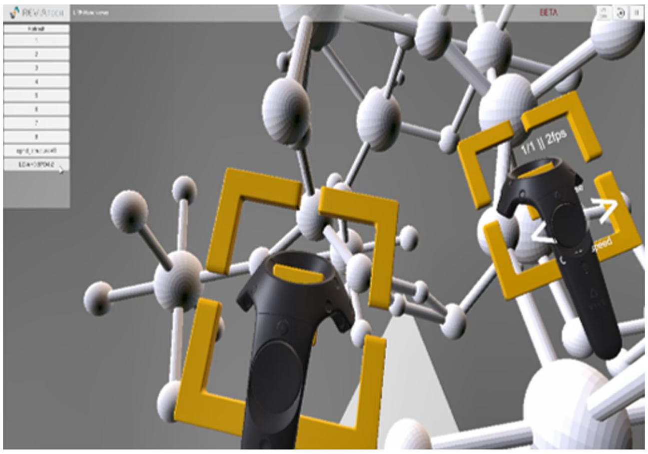

Figure 12. Snapshot of *Nanoviewer VR* when manipulating a crystal ($Li_2V(H_{0.5}PO_4)_2$) in the figure). Corresponding video provided in the Supporting Information.

Figure 13. A student using the Nanoviewer VR serious game. What is seen in the VR environment is projected in a screen to allow others to see as well.

Nanoviewer VR constitutes also a great tool for performing battery research. For instance, it helps scientists from our laboratory (LRCS) to visualize in an immersive and interactive way composite electrode mesostructures. Such images are arising either from CGMD simulations or from micro and nano computer tomography. It helps them to evaluate the quality of the segmentations (aiming to separate active material from CBD and pore phases), to assess the anisotropy of the electrodes and the heterogeneity of the materials location inside. The latter is of particular interest to analyze the influence of the manufacturing process on the homogeneity of the electrodes. Recently, *Nanoviewer VR* was extended to visualize videos in an immersive way, like CGMD particles trajectories for instance (to analyze for example the effect of the solvent evaporation dynamics on the final electrode mesostructure). Despite its intensive use by us in battery research, the software is very flexible to be used in other applications: for example, mathematics and organic chemistry colleagues already manifested their interest to use it to visualize complex 3D-dimensional mathematical functions and organic molecules.

2.4. The Great Li-Air Escapade VR Serious Game

As mentioned in the introduction (section 1), LOBs, also called lithium-air batteries, have attracted a significant interest for electric transportation, in view of their high energy density and high theoretical capacity, even though the aforementioned electrolyte stability and rechargeability issues make them very far away from commercialization.[60] A typical LOB cell consists of an anode (*e.g.*, lithium metal foil), an aprotic electrolyte with dissolved lithium salt, and a porous O_2-rich cathode with a large surface area (Figure 14a). During discharge lithium oxidizes in the anode giving Li^+ in the electrolyte. Electrons flow through an external circuit and Li^+ ions migrate from the anode to the cathode, where oxygen is reduced and Li_2O_2 is formed within the pores of the cathode electrode. The detailed mechanism leading to the formation of Li_2O_2 (oxygen reduction reaction -ORR-), and implicating $LiO_{2(sol)}$ as intermediate reaction specie has been widely discussed in the literature.[61–62] Li_2O_2, which is insoluble in the solvent, has very poor electron conductivity. It is believed that a solution phase reaction leads to the formation of large Li_2O_2 toroidal particles, while an

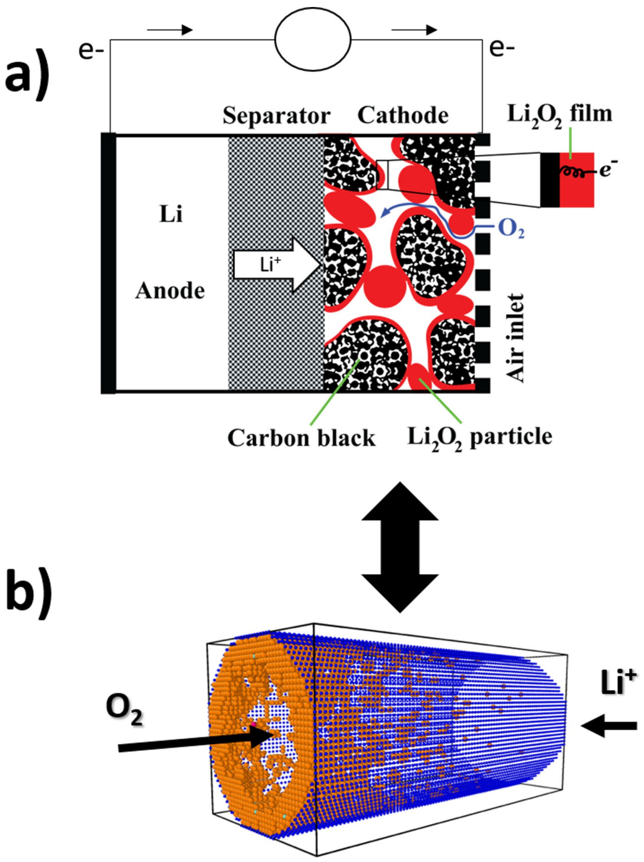

Figure 14. a) Schematic of a discharging LOB; b) simplified (cylindrical) representation of a LOB cathode in *The Great Li–Air Escapade VR* serious game (the forming Li_2O_2 upon discharge is represented in orange color; the influxes of O_2 and Li^+ are also indicated).

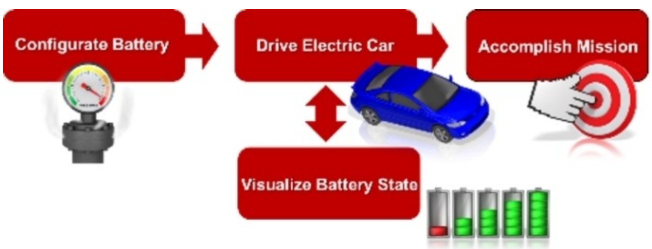

Figure 15. Flow Chart of *The Great Li–Air Escapade VR* serious game.

electrode surface reaction leads to the Li_2O_2 formation of dense thin film on the pore walls. In both ways, the amount of Li_2O_2 accumulates along the discharge, and leads to the passivation of the electrode surface and pores clogging towards Li^+ and oxygen transport, hence limiting the cell capacity.

In order to ease the understanding by students of the aforementioned complex operation principles of LOBs upon discharge, in 2016 we have designed and developed *The Great Li–Air Escapade VR*, an interactive and immersive VR serious game simulating the behavior of a LOB powering an EV which is driven by the player in a virtual city. The overall workflow of the game is presented in Figure 15. Before starting, the player is faced to an opening menu where she/he is requested to configure the battery, namely choosing a cylindrical pore radius (10, 20, 30, 40 and 50 nm), the O_2 pressure (1, 1.5, 2 bars) and the level of difficulty (easy, medium, hard) (Figure 16a). The level of difficulty impacts the number of police cars which will move randomly in the streets of the virtual city. After making these choices, the player can start playing by pushing the "start" button. The aim is to drive the EV in order to collect three gifts randomly distributed in the virtual city, in the shortest time as possible, by escaping from the police cars and by avoiding the LOB to be fully discharged (Figure 16b). While driving the virtual car, the player can see the cylindrical pore with the forming Li_2O_2 "floating" in the sky of the virtual city which allows her/him to track the state of charge of the LOB (Figure 16b). The player also sees a clock counting the game time and a porosity counter (porosity decreases with the depth of discharge).

The cylindrical pore represents a geometrical simplification of the actual porous mesostructure of a LOB cathode, to provide the students with a straight-forward impression of the implications of the Li_2O_2 formation mechanism depending on their way of driving the EV. Li_2O_2 is represented in orange color and its formation and spatial localization along the radius and the length of the cylinder is controlled via a lookup table interpolating values pre-calculated using a kinetic Monte Carlo (kMC) model reported by us elsewhere.[63–64] A lookup table is a data structure stored in the computer memory which is used to replace a calculation by a simple operation of consultation. It associates input and output values through numerical interpolation. The concerned kMC model resolves the detailed

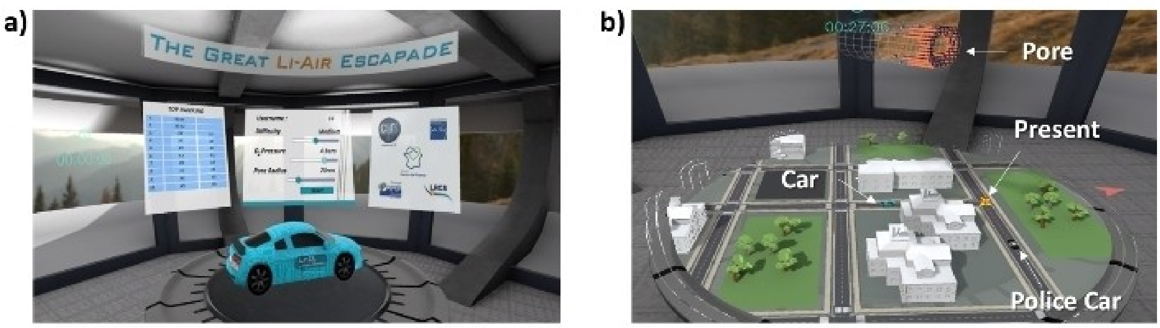

Figure 16. Snapshots of *The Great Li–Air Escapade VR* serious game: a) start menu; b) driving the car in the virtual city, where one can see the clock, the pore, the car, a gift and a police car in the virtual city. Corresponding video available in the Supporting Information.

Concepts
doi.org/10.1002/batt.202000120

electrochemical reaction steps and transport processes involving Li^+, $O_{2(sol)}$ and $LiO_{2(sol)}$ in the formation mechanism of Li_2O_2. This includes also the pore wall passivation by Li_2O_2, pore volume clogging and electronic tunneling effects as described in Ref. [63]. The latter captures the fact that the passivating film of Li_2O_2 can still conduct electrons by quantum tunneling until reaches a thickness of 10 nm for which it becomes non-conductive. The kMC model also captures the heterogeneous Li_2O_2 formation along the pore channel length: Li_2O_2 forms closer to the O_2 inlet, because typically O_2 transport is slower in LOB electrolytes than Li^+ ions.[65–66] Examples of calculated Li_2O_2 distributions at two depths of discharge and for different pore radius are reported in Figure 17. It can be noticed that the pore with 10 nm radius becomes totally clogged at the end of discharge whereas larger pores not, because Li_2O_2 film is assumed to stop growing when it reaches 10 nm thickness. For the larger pores it is underlined that the film passivation leads to the full discharge of the LOB.

The lookup table procedure is adopted because it is hard to implement real-time kMC simulations in the game without penalizing the overall computational cost of the VR environment. The lookup table has been built by running offline kMC simulations, which allows extracting the pore geometry evolution as function of discharge history and pore size. With employing this lookup table, *The Great Li–Air Escapade VR* achieves to show the formation of Li_2O_2 depending on the EV driving conditions. For instance, more frequently the EV is moving, faster will be the growth of Li_2O_2 in the cylindrical channel. The O_2 pressure chosen by the player in the start menu is another parameter that controls the speed of formation of Li_2O_2: higher O_2 pressures will imply faster formation of Li_2O_2, even though more powerful the EV will be (*i.e.* it will have faster acceleration-rates). *The Great Li-Air Escapade VR* constitutes a very interesting concept to allow carrying out computational modeling without direct access to the code, but instead, through the use of a user friendly (VR) interface: players they do not see the kMC-generated lookup table, but only the results.

The game has been designed to be used with an Xbox gamepad, as shown in Figure 18. The analog sticks are used to steer the car and to navigate the menus, the left shoulder button reverses the direction of the car and the right shoulder button accelerates the car. This is to favor the easiness of the use of the game, by considering that a significant number of students have already experience with classical Xbox car games. In order to help players to orientate themselves in their tasks, red arrows appear in the virtual city indicating the directions where police cars are localized at each time, while green arrows indicate the direction where it is localized the next gift to collect (see video of the serious game in the Supporting Information).

Thanks to the kMC-generated lookup table embedded in the game, *The Great Li–Air Escapade* allows students to understand the LOB operation principles by experimenting with the different possible parameterizations at the beginning of the game as well as with the different ways of driving the EV (Figure 19). For instance, for a small pore chosen and frequent accelerations, the capacity of the virtual LOB will be small (as pore gets clogged with Li_2O_2 quickly), whereas with a larger pore and less accelerations capacity will be longer. Still, even with large pores, if acceleration is frequent, capacity will go down quickly because of the Li_2O_2 tunneling effects discussed above. Depending of the chosen level of difficulty and way of behaving in the game, typical duration of a successful game (*i.e.*, where the player succeeds collecting the three gifts) is comprised between *ca.* 1 and 5 minutes.

A limitation of this game was pointed out by students while playing with it: the game does not consider the EV momentum. The EV car stops moving "drastically' when the LOB reaches a fully discharged state. As a consequence, a player very close to collect her/his third (and last) gift may lose the game because

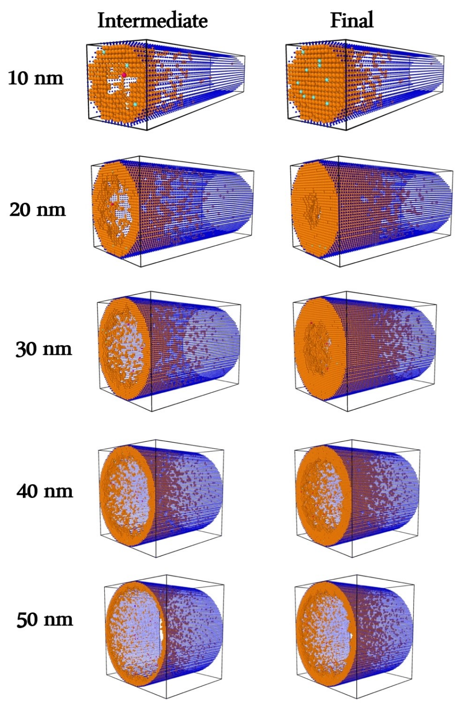

Figure 17. Calculated Li_2O_2 distribution using kMC simulations at intermediate and final depths of discharge for different pore sizes (O_2 entering from the left and Li^+ from the right of the channels). The calculated dynamics is used to set a lookup table integrated in the VR environment (illustrative video provided in the Supporting Information).

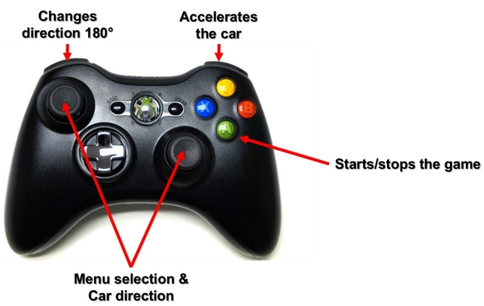

Figure 18. The Xbox commands of the VR serious games *The Great Li–Air Escapade VR* and *The Great EV Escapade VR* (for the latter, see below).

Figure 19. A student playing *The Great Li–Air Escapade VR* serious game.

Figure 20. The virtual country side map of *The Great EV Escapade VR* serious game. The driven EV and the vans move on the roads only (in white color) and the gifts are randomly located on the roads. The blue color represents the virtual sea and two virtual lakes. The dark green color represents the virtual hills.

the EV stops moving whereas momentum after a last boost may permit her/him by the motion momentum to collect it. This limitation motivated us to develop a new generation of game considering more realistic features of the EV motion mechanics as well as more realistic representation of the LOB cathode electrode, as well as the possibility to use also other two battery technologies to compare the performances (LIBs and LSBs): *The Great EV Escapade VR* serious game was born.

2.5. The Great EV Escapade VR Serious Game

The Great EV Escapade VR serious game is supported on the same concept as *The Great Li–Air Escapade VR*: the player has to collect three gifts randomly placed in a virtual environment, within a limited time, and by escaping from black vans. However, it introduces several significant improvements:

- in the start menu the player can choose between a LIB, a LSB or a LOB to power her/his EV. For the case of the LOB, the player can still configure the O_2 pressure applied to the cathode;
- the player can choose between the virtual city map (identical to the one in *The Great Li–Air Escapade VR*) or a country side map which includes bridges and hills (Figure 20);
- the game accounts for the effect of gravity, momentum, friction and inertia on the EV motion. The associated mechanical laws are fully tunable in the game through a Python script which can be configured before launching the game in the hosting computer;
- for each of the three types of batteries, while driving the EV, the cathodes are represented with realistically evolving mesostructures floating in the virtual sky. The pristine cathode mesostructures (before discharge) mimic a $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ -based electrode for the LIB, a sulfur-loaded carbon-based electrode for the case of the LSB and a carbon-based electrode for the case of the LOB. The electrode mesostructures were generated from experimental parameters (porosity) using the Geodict computational software, similarly to the generation of the electrode mesostructures used in the *Tortuosity VR* serious game.

The representation of the evolution of the cathode mesostructures in the game follows a similar strategy as in *The Great Li–Air Escapade VR*: lookup tables are built based on calculations carried out by using simplified versions of models previously reported by us.[56,64, 67] In the LSB case, the (carbon-based) cathode evolution representation is more complex (Figure 21). In a LSB cathode upon cell discharge, solid S_8 initially present in the cathode, first dissolves in the electrolyte, and then it is sequentially reduced to polysulfides S_8^{2-}, S_6^{2-}, S_4^{2-}, S_2^{2-} and S^{2-}. Li_2S_2 and Li_2S form and precipitate in the cathode pores dealing to their clogging and the pores walls passivation slowing down the S_8 reduction kinetics. In the game, sulfur particles initially present in the cathode pores are represented as cubes in yellow color randomly localized, and the precipitates are represented as green spheres forming gradually and randomly locating on the carbon surface upon the LSB cell discharge. Pre-calculated lookup tables using kMC

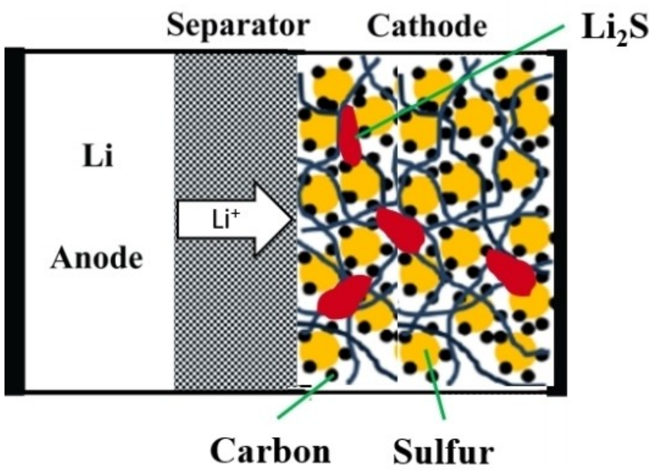

Figure 21. A scheme of a LSB cell and its discharging cathode.

simulations can be used to describe sulfur particles dissolution, polysulfides formation and Li_2S precipitation.[67]

The Li^+ intercalation process in a $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ -based cathode upon the LIB discharge is represented by a gradually and spatially localized changing color in the cathode mesostructure (ranging from green -pristine cathode- towards red-fully intercalated electrode). In the LOB case, the Li_2O_2 distribution in a carbon matrix-based cathode is arising from a random location algorithm.

The lookup tables describing the discharge of the cathodes are flexible and can be tuned, for example in regards to their speed of discharge (in the starting menu and in a Python script). The mechanical properties of the EV (*e.g.*, degree of friction with the roads) can be also adjusted through a Python script before starting to play. This provides the opportunity to use *The Great EV Escapade VR* as a true multiphysics simulator encompassing electrochemistry and mechanical simulators, without any requirement of programming skills. Again, this presents strong benefits for education and for battery research.

Similarly to *The Li–Air Great Escapade VR*, this serious game requires good movement coordination, as the player has to accomplish her/his mission by avoiding the battery cell to be fully discharged, by regularly checking the mesostructure flying on the sky (Figure 22).

Depending of the chosen level of difficulty (number of vans randomly moving in the virtual city or in the country side), the way of behaving in the game, the chosen type of battery (battery autonomies range like LIB < LSB < LOB to represent theoretical capacities)[8] and the chosen discharge rate, typical duration of a successful game (*i.e.* where the player succeeds collecting the three gifts) is comprised between *ca.* 1 and 5 minutes.

The Great EV Escapade VR allows putting students in the situation of driving an EV with battery technologies that are not yet commercial for automotive applications (LSBs), or that still present enormous technical challenges (LOBs), and compare their theoretical performance with the ones achievable with LIBs (Figure 23). Their capacities still depend on the way of driving the EV (more frequent is the acceleration, faster the battery will discharge). Finally, it can be noticed that this serious game does not represent the behavior of the anode and does not allow recharging the EV. The latter aspects were integrated in the most evolved and the most recent VR serious game we have created (still in prototype stage): *Smart Grid*

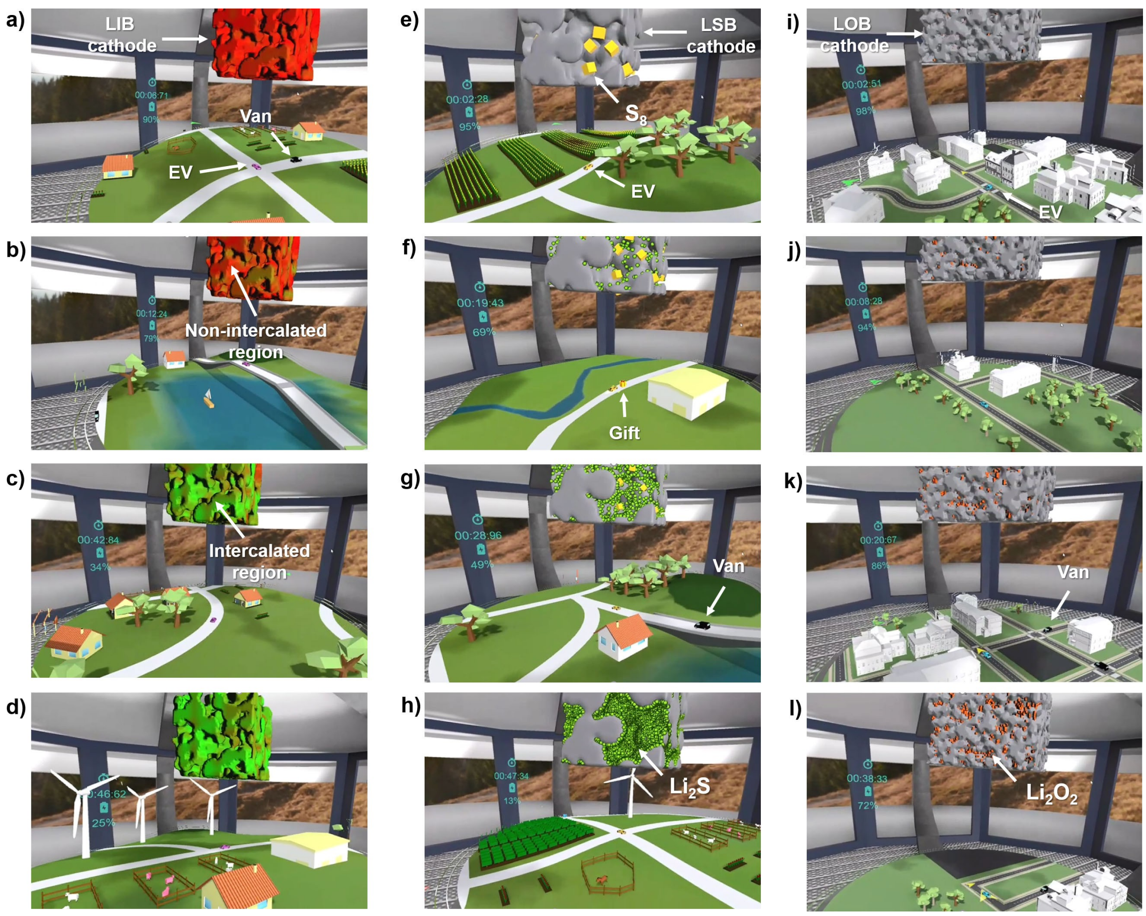

Figure 22. *The EV Great Escapade VR* serious game. a-d) Snapshots of a game driving a LIB-powered EV in the virtual country side; e-h) snaphots of a game driving a LSB-powered EV in the virtual country side; i-l) snapshots of a game driving a LOB-powered EV in the virtual city. Details of state of operation of the cathodes for the three battery cases are shown. Corresponding video provided in the Supporting Information.

Figure 23. A student playing *The Great EV Escapade VR* serious game.

Mixed Reality (*Smart Grid MR*), presented in the following section.

2.6. Smart Grid MR Serious Game

A smart grid is an electricity grid enhanced by information technology for interlinked and automated electricity generation, transmission, distribution and control.[68–69] It encompasses electricity sources (*e.g.*, renewables), energy sinks (*e.g.*, EV recharge stations, houses, industry) and stationary energy storage to ensure a continuous electricity provision when variable renewable energies are implicated (Figure 24). A smart grid operation can be seen, within the scope of the game theory, as a collective game involving cooperation (*e.g.*, ensemble of electricity generators) and competition (*e.g.*, electricity provision vs. consumption), from which complex behavior emerges.[70–71]

In order to ease the understanding by students of the interplay between electricity generation, distribution, storage and consumption, in 2019 we have designed and developed the *Smart Grid MR* serious game. This serious game proposes a collaborative platform mixing VR environment with real objects, constituting a "mixed reality" concept (for which the acronym "MR" stands for) (Figure 25).

In such a platform one player evolves in the VR environment by driving an EV in a virtual 3D-map, containing both urban and country side zones (Figure 26b). The roads in the map are two-way (in contrast to *The Great Escapade* games) and contain recharge stations, bridges and barriers appearing and closing a road randomly. Similarly to *The Great Escapade* games, vans move randomly on the roads and aim to catch the EV. The player also has to collect gifts, which randomly appear in the virtual map. In contrast to the EV serious games described above, in here the number of presents is unlimited, therefore the player goal is collecting as much as she/he can before she/he loses. More gifts are collected, more difficult becomes the game as the number of vans and the frequency of appearance of barriers become higher. The player can lose if she/he is captured by the vans or if the battery in the EV becomes fully discharged. To avoid the latter, the VR player can park for few seconds in one of the recharge stations and recharge the battery (Figure 26c). The electricity in the recharge stations is provided by a stationary redox flow battery localized in the virtual map. Such a stationary battery can be recharged with the virtual electricity produced by a group of players acting on real 3D-printed objects (Figure 26d) connected to the VR software via Bluetooth. Such objects consist of

- one wind turbine that can be activated with real wind (*e.g.*, by blowing on or by producing wind by moving a piece of paperboard). When moving, the turbine produces electricity stored in the stationary battery;
- a water funnel that when throwing water in it makes raining in the virtual environment. The rain fills a water dam in the virtual environment: when the water reaches a critical height, the dam starts to produce electricity that is sent to the stationary battery (until water reaches a height under the critical level);
- a solar panel that can be activated with the flash light from mobile phones. Again, the produced virtual electricity is sent into the stationary battery.

There is also a virtual tidal power station in the VR environment, visible on the 3D map, that creates continuous energy from the nearby sea shore. This station is therefore not activated by the players, but it can be turned off through a Python script.

The solar panel cannot produce electricity when it is raining in the virtual city and vice-versa. The degree of production of

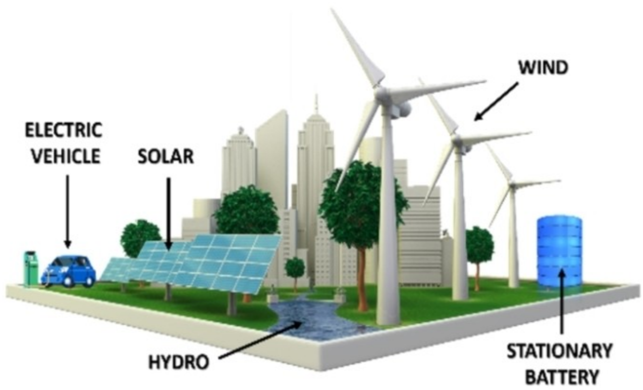

Figure 24. Constituents of an electric smart grid.

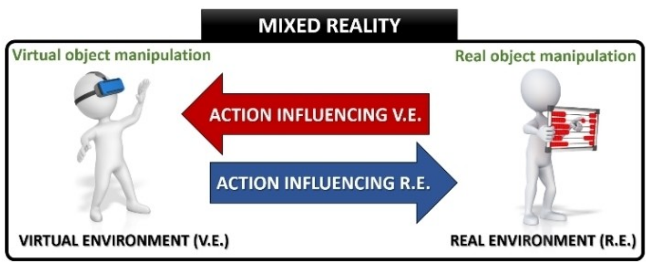

Figure 25. Mixed reality concept.

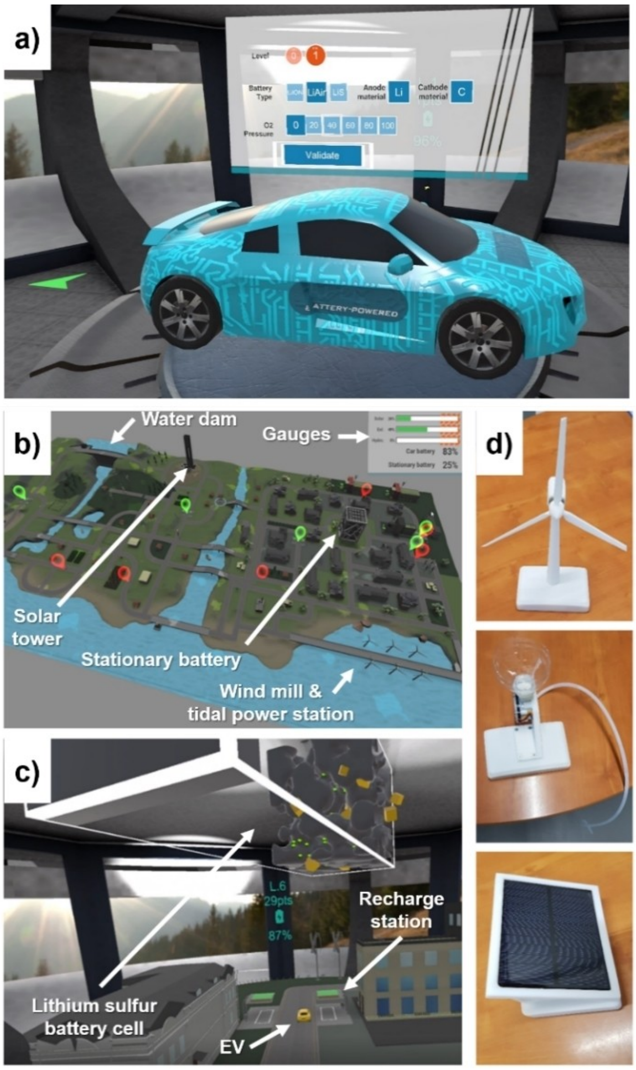

Figure 26. Prototype of the *Smart Grid MR* serious game developed by us: a) one of the starting menus (case of LOB configuration); b) virtual city map showing the location of EV recharge stations (in green) and of the vans (in red), and also the electrical energy production gauges by different sources (wind, solar, hydro) activated by the students in the real world; c) viewpoint by the student wearing the headset and driving the EV; d) 3D-printed devices used by the students in the real world to generate electricity (connected by Bluetooth to the Virtual Environment).

electricity through the three real devices can be followed through three gauges (top right in the Figure 26b). If an energy source reaches the orange zone of the gauge, the energy produced is not injected anymore in the stationary battery during 10 seconds. The worst scenario for the EV driver would be that her/his battery and the stationary battery are fully discharged: in that situation, the player will also lose the game as she/he cannot recharge the EV while parking in the recharge stations. The game then needs for a good coordination or collaboration between the EV driver and the players generating the virtual electricity (under the constraint of solar vs. rain mentioned above). The VR player only sees the virtual environment (Figure 26c) whereas the other players can see, through a 2D screen, either what the VR player sees or the virtual map all together (Figure 26b) (the two views can be switched between them by pushing Alt command in the computer keyboard). In the virtual map view, red icons indicate the instantaneous position of the vans, the fixed light green icons the localization of the recharge stations whereas the mobile dark green icon indicates the instantaneous position of the EV driven by the VR player.

An interesting feature of *Smart Grid MR* is that the "battery technology" menu has been extended. As previously, the user can choose between LIBs, LSBs and LOBs but for each technology, more options are now available (Figure 26a). For LIBs, the active materials of both anode and cathode (*e.g.*, graphite or lithium titanium oxide for the anode, lithium iron phosphate or lithium nickel-manganese-cobalt oxide for the cathode) can be chosen, leading to different battery capacities. In the LSBs case, the sulfur loading can be tuned and finally for LOBs cathodes, the O_2 pressure is allowed to be changed by the user. The possible choices of materials and conditions in the start menu are fully configurable through a Python script: this is thought to include real research results (real capacities vs. materials chemistries or vs. electrode configurations). While driving the EV, the VR player can see the full cell (anode/separator/cathode) floating in the air, with electrode mesostructure evolutions represented in a similar way to the ones described in *The Great EV Escapade VR* serious game. Such evolutions allow the RV player to track the state of charge of her/his chosen battery.

Another interesting feature is that *Smart Grid MR* allows recording a game status (as a multiplayer profile) and continuing it later. The players "level" label in the game increases with the number of collected gifts. As there is not limit in the number of possible collected gifts, therefore players can decide to stop playing at any time and continue from their latest reached level later. This is in particular useful when a professor wants their students to split the use of the serious game along different practice days.

Smart Grid MR characteristics are very useful for training students about smart grid concepts, battery materials concepts, the importance to find a good balance between EV battery characteristics, electricity production by renewables and storage and also to improve their collaboration and team work skills (Figure 27). It can also constitute a great tool for research, to investigate the working principles of smart grids: the links between the amounts of electricity produced and way of acting on the 3D-printed devices are fully parameterizable through a Python script. The same applies for the battery materials as mentioned above, the stationary battery capacity and for the EV motion properties (mass, friction, etc.).

We have recently started implementing new functionalities to the game, with new 3D-printed devices, including more wind turbines, electricity consumption devices (houses, shops, industries), electricity distribution devices (allowing to manage the electricity flow between the electricity generators, the stationary battery, the electricity consumers and the recharge stations) and a fortune wheel generating randomly electricity production disruptions. Possibilities of scenarios to study players' interactions (collaboration vs. competition) become then very wide.

Figure 27. Utilization of the *Smart Grid MR* serious game. Both the virtual map and what is being seen by the EV driver can be show in the screen alternatively (Photo taken by Cyril Fresillon, Photothèque CNRS/LRCS, Copyright CNRS. Reproduced with permission).

3. Usage and Impact

Since their creation, we have been using our serious games as illustrations in lectures and for practices at the University level, and as demonstrations in seminars, international conferences and popular science events. Some of the serious games (*Tortuosity VR* and *Nanoviewer VR*) have been also used for research purposes (to visualize electrode mesostructures and calculate their tortuosity). Users include:

- in average 20 students/year of the MSc. "Chemistry" (CD MAT) and "Erasmus+ Materials for Energy Storage and Conversion" (MESC+)[72] of the Université de Picardie Jules Verne (UPJV) in Amiens, France;
- in average 20 students/year of the UPJV Chemistry Bachelor in Amiens, France;
- 25 students of the UPJV Psychology Master (year 2018), in Amiens, France;
- in average 30 MSc. students/year of the IFP School,[73] in Rueil Malmaison, France;
- more than 100 scientists/engineers in international conferences and seminars (*e.g.*, MODVAL conference – Germany 2019, Workshop "Theory Meets Industry" – France 2019, BATMAN Summer School – Denmark 2019; Chalmers University of Technology – Sweden 2019, CIC Energigune – Spain 2019, etc.);
- until now, >500 persons from the general public (kids, adolescents, adults, seniors) (*e.g.*, popular science events: Pint of Science festival,[74] Fête de la Science,[75] in several French cities including Amiens, Beauvais and Boulogne-sur-Mer);
- we have been also invited to present our VR serious games concept to the French Minister of High Education and Research, Frédérique Vidal (May 14, 2018, Amiens, France) and to the President of France, Emmanuel Macron (November 21, 2019, Amiens, France).[76]

This diversity of audiences addressed allowed building a very rich database to evaluate how our serious games motivate, engage and ease the understanding of the complex concepts involved in the battery field depending on the type of audience (see a selection of photos and videos in the Supporting Information).

Before engaging students or the general public to play, we use to explain the aspects that are going to be exercised or demonstrated using our VR serious games. Such explanations can be with Power Point presentation support in the case of science festivals, scientific seminars or lectures at the University. Then we proceed with a demonstration by ourselves of the working principles of the concerned serious game, and then we engage the public to play with. All audiences show very significant enthusiasm as soon as we announce that we are going to make demonstrations or practices using VR.

In some cases (*e.g.*, lectures with the MESC+ and CD Mat master students) we have organized World Cup-style competitions using *Tortuosity VR* (2018 and 2019), *Nanoviewer VR* (2017 and 2018), *The Great Li–Air Escapade VR* (2016 and 2017) and *The Great EV Escapade VR* (2018 and 2019) and give prizes (*e.g.*, scientific books or scaled-up 3D plastic-printed electrodes) to the students performing the best (*e.g.*, taking the shortest time to collect the gifts in *The Great Escapade* serious games). These students' competitions were organized in slots of 30 minutes duration after each lecture of 1 h30 covering theoretical aspects of computational modeling of batteries, their materials and operation principles, etc. Though the MESC+ and CD Mat MSc. students have usually the basic knowledge of chemistry, most of them are not familiar with computational modeling in the field of batteries.

Still regarding university lectures, three types of impact studies have been conducted with our VR serious games, for which the main observations are summarized next. The first aimed at collecting the professors' feedback (professors using the games in their lectures) through semi-directed interviews. Results suggested that VR offer a better interactivity between professors and students and between students themselves, compared to presentations in screens including videos, or practices using mathematical models coded in software like MATLAB. This is because students are confronted to games in unusual environments which offer the opportunity to feel "from inside" the materials, electrodes or the impact of the way of driving the EV on the batteries behavior and performance. The second study aimed at collecting the students' feedback through collective interviews and by analyzing video-recorded students' behavior while playing. Our VR serious games are globally perceived as "easy to use" and students strongly appreciate their interactivity. Concerning the usefulness of our VR serious games in general and their insertion in university lectures, students' feedback are very positive, as they consider them as a very good gateway for novices towards detailed battery research.[40] Students find that our VR games make the lectures more dynamic and more interactive. The link between theory and practice can be better performed according to students. The third study aimed at quantifying the pedagogical value of our VR serious games. It results that these games allow to identify the students who have acquired concepts taught in lectures and those who are in difficulty. Therefore, the added value of these VR games is twofold: to experiment in VR with the concepts seen in the lectures in order to validate the acquired knowledge and to identify through the serious games the students having difficulties to make them to revise the concepts. The immersive and interactive VR characters were also shown to allow students to better understand three-dimensional concepts (such as crystal symmetries or electrodes anisotropies).[40]

We have also studied in deep how *Nanoviewer VR* impacts learning performances and motivation by students.[41] For that purpose, psychology undergraduate students (*i.e.*, no battery-specialists), were split in two groups, one using VR (experimental group) to visualize and interact with a LIB electrode mesostructure (cf. Figure 13), and one having access to images under different perspectives of the same electrode printed on paper (control group). The two groups have been requested to count and to give an estimation of the number of "large particles" (*i.e.*, representing the active material particles) present in the LIB electrode mesostructure. Results showed that *Nanoviewer VR* allow participants a better efficiency in providing the right answer than participants of the control group. In terms of motivation, *Nanoviewer VR* created a higher intrinsic motivation compared to the control group.

Our VR serious games have been of crucial importance to expand students' horizon of knowledge. For instance, *Crystal VR* rises students' interest by crystallography and the mathematical operations behind, whereas *Tortuosity VR* make students realize about the composite electrodes' tortuosity anisotropy and its implications in terms of lithium ion transport properties. Serious games like *The Great Escapade* and *Smart Grid MR* also strength their awareness of cooperation by encouraging multidisciplinary discussion.

We believe that our VR serious games have a strategic dimension in terms of training, but also in terms of science popularization and research. They describe in immersive and interactive way battery materials, electrodes and their operation principles thanks to the use of mathematical operations, mathematical models and results, some of the latter (*e.g.*, composite electrode mesostructures) obtained in research projects such as ARTISTIC.[77] Then our serious games also act as an innovative "show room" interface to present project results to students and to the general public, without requiring for them to have knowledge on programming or other scientific skills. Players learn about batteries by "doing", through their immersion and interaction in the VR environment. This ease our way of communicating about our research activities, and rises the awareness of the large public.

Thanks to the strong collaboration between chemists, physicists, engineers, informaticians, psychologists and ergonomists in our team, we optimize the integration of these technologies in our lectures and in the demonstrations to the general public. Indeed, our games have shown to be very intuitive for use of a wide spectrum of ages, from children to adults (see the Supporting Information). They engage very significantly their interest as manifested by their frequent asked questions. Players have suggested improvements of our VR serious games that we have implemented: *e.g.*, the consideration of the EV momentum and the gravity effects in *The Great EV Escapade* or an improvement of the Xbox controllers in the *Smart Grid MR* serious game.

Our VR serious games allow people to better understand complex concepts in materials science, batteries and mathematical modeling, which are difficult to communicate by using only static 2D projections in PowerPoint presentations or in video format in computer screens. These VR serious games have strong potential to support also battery R&D: *Nanoviewer VR* and *Tortuosity VR* are frequently used by our laboratory researchers to analyze materials and composite electrode meso structures, and *The Great Escapade* and *Smart Grid MR* serious games can reveal to be great simulation platforms to test battery and electric grid mathematical models.

4. Conclusions

In this Concept we presented six immersive and interactive virtual reality (VR) "serious games" that we have developed for battery education at the university and in science popularization events:

- *Crystal VR*, which allows, through two virtual workshops, learning about symmetry operations and building crystal structures with some of the most common atoms used in battery active materials;
- *Tortuosity VR*, which allows flying through battery porous composite electrodes and calculating the associated tortuosities along the X, Y and Z spatial directions;
- *Nanoviewer VR*, which allows visualizing and interacting with materials at multiple scales from crystals to composite electrodes either coming from computational simulations or from tomography characterizations;
- *The Great Li–Air Escapade VR, which allows* driving a LOB-powered electric car in a virtual city to accomplish the mission of collecting three gifts by escaping from police cars at the shortest time as possible;
- *The Great EV Escapade VR*, which allows driving a battery-powered electric car in a virtual map (city or country side) to accomplish the mission of collecting three gifts by escaping from vans at the shortest time as possible. Before starting, players can choose their type of battery (LIB, LSB or LOB) and can visualize the porous electrode state (and therefore the battery cell state of charge) while driving the car;
- *Smart Grid MR*, supported on the mixed reality concept, which allows simultaneous interaction between multiple players. One of the players drive the electric car in a virtual environment as in *The Great Escapade* serious games, and the others generate electricity by interacting with real 3D-printed objects (wind turbine, hydro funnel, solar panel). Such electricity is stored in a stationary battery in the virtual environment which feeds recharge stations where the first player can recharge the car. The car driver can choose among different types of batteries which can be parameterized before starting the game. The overall goal of this

game is to collect as much gifts as possible without being captured by randomly moving vans.

We have decided to not fully describe the details in this Concept, but we have observed and measured several times the educational effects of our VR serious games on the players (motivation, ease of learning, interactivity, ergonomics, etc.) using complementary approaches, *e.g.*, quasi-experiments by comparing a traditional teaching situation (*i.e.*, without VR) and a situation using the VR serious games: for these two situations, we measured the memorization, the acquisition and the understanding of the targeted concepts as well as the commitment and the motivation, via questionnaires and interviews. We have observed these pedagogical situations, audio-visually recorded for careful analysis, with particular attention paid to the behavior of the players when evolving in the VR environments. The results allow us to optimize the integration and use of the VR serious games in lectures and in popular science events. After four years of intensive use of our VR serious games in university lectures for undergraduate and MSc. levels, we can affirm that students feel more engaged and motivated by this "learning by doing" concept than traditional lectures without use of VR.

We plan to make these serious games available for the community through a dedicated "Battery Education" webpage we are going to create.

Even if we did not find any player who complained about cybersickness or mental overloading while playing with our VR serious games, in the near future we are going to study these aspects in more detail in order to optimize even more our serious games ergonomics. We also think that VR can be an aid for students who learn more effectively through seeing and doing, rather than listening. It would be interesting to study the effect of these VR games on students with different learning styles.

Other perspectives of extension of our VR-related work include the combination of VR with artificial intelligence for personalized training. The VR concept introduced in this article also paves the way towards digital twins of batteries and processes (*e.g.*, battery manufacturing plants), as wells as to a next generation of computational tools making computational modeling research accessible to a wide spectrum of researchers (including the non-expert ones), beyond also batteries. The idea of performing battery research by "playing" comforts the famous quote, known for being from Albert Einstein, which says that "*play is the highest form of research*".[78]

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Conflict of Interest

The authors declare no conflict of interest.

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