Institution: University of Liverpool		
Unit of Assessment: 8		
Title of case study: ChemTube3D: a worldwide Open Educational Resource		
Period when the underpinning research was undertaken: 2004-current		
Details of staff conducting the underpinning research from the submitting unit:		
Name(s):	**Role(s) (e.g. job title):**	**Period(s) employed by submitting HEI:**
Prof. Nick Greeves	Professor Director of Teaching	1989-current
Prof. Matt Rosseinsky	Professor	1999-current
Prof. Andrew Cooper	Professor	1999-current
Prof. Laurence Hardwick	Professor	2011-current
Prof. Mathias Brust	Professor	1998-current
Period when the claimed impact occurred: 1/8/13-31/12/20		
Is this case study continued from a case study submitted in 2014? No		

1. Summary of the impact

ChemTube3D is a web-based resource that delivers free interactive three-dimensional animated chemistry visualisations to educators, students, and members of the public. ChemTube3D has delivered profound impacts on understanding, learning and participation within chemistry. Public interest and engagement in research has been stimulated and the delivery and design of curriculum within schools and HEI's has been significantly enhanced. This is evidenced by:

(i) >5 million users (13.8 million page views) with 58% in the target age range (18-24) in the REF period
(ii) Use in schools/HEI's worldwide with the site embedded in >80 virtual learning environments and 32000 direct links to pages of ChemTube3D from other web sites.
(iii) #1 in Google searches (Dec 2020) for >200 terms including "chemistry animations".
(iv) Adopted by Oxford University Press into the sector leading undergraduate textbooks and incorporated into A-level schemes of work.

2. Underpinning research

ChemTube3D.com is an Open Educational Resource (OER) comprised of over 2400 pages containing interactive 3D animations and structures, with supporting information. ChemTube3D is aimed at students and educators at school/college and University alike as well as interested members of the public.

ChemTube3D was developed as a direct result of the EPSRC supported research carried out in the Rosseinsky and Cooper groups during the Complex Materials Discovery Portfolio Partnership (2004-2010 EP/C511794/1). This research programme developed new solid-state inorganic and polymer materials with breakthroughs including the isolation of the molecular superconductor Cs_3C_{60} [3.1], conjugated microporous polymers with specific surface areas of up to 834 $m^2\ g^{-1}$ [3.2] and peptide-based metal organic frameworks [3.3]. During this programme there was a growing realisation amongst the PIs, and their colleagues across the Chemistry department of the power of interactive 3D computer visualisation techniques within materials chemistry discovery. 3D models became routinely used within the research programme to enable an understanding of the complex structures being made. It became apparent that to enable public engagement with the ongoing research and to facilitate the teaching of complex structures and chemical concepts, 3D visualisation would be required. At the time, these techniques were virtually invisible in the undergraduate chemistry curriculum in the UK. As a consequence, the Liverpool chemistry team led by Greeves, funded by the outreach component of EP/C511794/1, developed a web-based visualisation resource, which was formally launched as ChemTube3D in 2008. Key to the concept of ChemTube3D was representing materials research advances in a way that facilitated engagement with the public and with undergraduates, going beyond the rather traditional structures that are customarily represented in such engagement.

The website, and subsequent apps (iPhone and Android), continue to be developed with a subsequent joint project between JISC and UoL (£100k, 2009-2010) called *iChem3D: Supporting lifelong learning: enhancing the value of interactive 3D chemistry* [5.2] leading to a much-improved web site in terms of user interface, animation functionality, and breadth of content and a further update of the site occurred in 2019. The site now covers some of the most important topics covered during an undergraduate chemistry degree and A level, making use of the visualisation approaches originally employed within the Complex Materials Discovery Portfolio Partnership. Research breakthroughs from our department are embedded and referenced within the material for use in undergraduate and A level teaching and the research led pages remain amongst the most popular with a small selection of examples including;

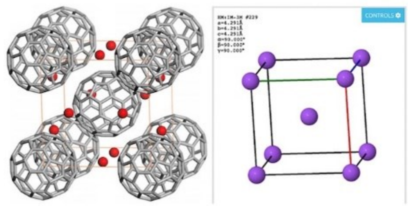

Fig 1. Cs_3C_{60} and body centred cubic structure from ChemTube3D

Molecular materials: Research from the Rosseinsky group (2004-2010 EP/C511794/1) led to Cs_3C_{60} being isolated, a superconductor with the highest T_c of any molecular material at 38 K [3.1]. It exhibits a simple body centred cubic packing of the fulleride anions and relates directly to the representations of sphere packing which led to the creation of the popular solid-state inorganic structure section which was specifically funded by the outreach component of this large grant.

Metal Organic Frameworks: Research from the Rosseinsky group (2009-2016 EP/H000925 and EP/J008834) lead to the discovery of a peptide-based porous 3D framework, ZnCar synthesized from Zn^{2+} and carnosine [3.3, 3.4]. Single-crystal X-ray diffraction showed that the ZnCar framework adapts to MeOH and H_2O guests because of the torsional flexibility of the main chain, while retaining the rigidity conferred by the Zn–imidazolate chains [3.3-3.4]. The ability to exchange guests and the flexibility of the structure is captured by animated pages showing the structural changes and these have since been expanded to cover a range of MOF structures.

Li ion batteries: Research from the Hardwick group (2013-2019, EP/K016954/1) explored the mechanisms of Li intercalation into graphite flakes [3.5] using in situ Raman spectroelectrochemistry. A series of pages devoted to the structures of important electrode and electrolyte solid-state materials was constructed including unique animations of the movement of Li ions within the materials.

Polymers: The Cooper group discovered conjugated microporous polymers that exhibit specific surface areas of up to 834 $m^2\ g^{-1}$ within EP/C511794/1 [3.2] and Chemtube3D is used to provide a powerful visualisation of the contrast between these conjugated microporous polymers and conventional polymers. As a result of this research the polymer section of the site was developed.

Gold nanoparticles: Based on protein folding considerations, the Brust group (BBSRC 26/E18028 and 26/B18374) group designed a pentapeptide ligand, which converts citrate-stabilized gold nanoparticles into extremely stable, water-soluble gold nanoparticles with some chemical properties analogous to those of proteins [3.6]. Pages illustrating polyhedral structures of gold nanoparticles and an animation showing encapsulation as part of a large section on gold nanoparticles were produced as a result of, and to communicate, this research.

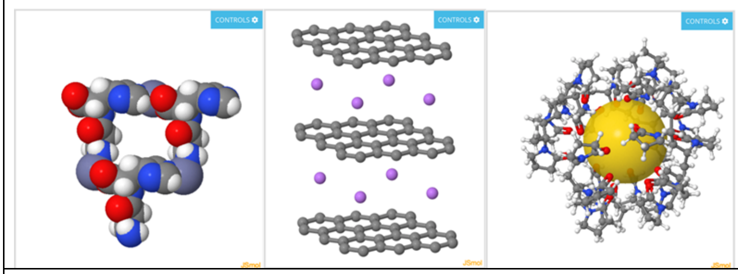

Fig 2. ZnCar pore animation, lithium intercalated in graphite and a polyamide encapsulated gold nanoparticle from ChemTube3D.

3. References to the research

3.1 Ganin, A. Y.; Takabayashi, Y.; Khimyak, Y. Z.; Margadonna, S.; Tamai, A.; Rosseinsky, M. J.; Prassides, K. Bulk Superconductivity at 38 K in a Molecular System. Nat. Mater. 2008, 7, 367-371. https://doi.org/10.1038/nmat2179.

3.2 Jiang, J.; Su, F.; Trewin, A.; Wood, C. D.; Campbell, N. L.; Niu, H.; Dickinson, C.; Ganin, A. Y.; Rosseinsky, M. J.; Khimyak, Y. Z.; et al. Conjugated Microporous Poly(aryleneethynylene) Networks. *Angew. Chemie - Int. Ed.* **2007**, 46 (45), 8574–8578. https://doi.org/10.1002/anie.200701595.

3.3 Katsoulidis, A. P.; Park, K. S.; Antypov, D.; Martí-Gastaldo, C.; Miller, G. J.; Warren, J. E.; Robertson, C. M.; Blanc, F.; Darling, G. R.; Berry, N. G.; et al. Guest-Adaptable and Water-Stable Peptide-Based Porous Materials by Imidazolate Side Chain Control. *Angew. Chemie - Int. Ed*. **2014**, 53 (1), 193–198. https://doi.org/10.1002/anie.201307074.

3.4 Vaidhyanathan, R.; Bradshaw, D.; Rebilly, J. N.; Barrio, J. P.; Gould, J. A.; Berry, N. G.; Rosseinsky, M. J. A Family of Nanoporous Materials Based on an Amino Acid Backbone. *Angew. Chemie - Int. Ed.* **2006**, 45 (39), 6495–6499. https://doi.org/10.1002/anie.200602242.

3.5 Zou, J.; Sole, C.; Drewett, N. E.; Velický, M.; Hardwick, L. J. In Situ Study of Li Intercalation into Highly Crystalline Graphitic Flakes of Varying Thicknesses. *J. Phys. Chem. Lett.* **2016**, 7 (21), 4291–4296. https://doi.org/10.1021/acs.jpclett.6b01886.

3.6 Lévy, R.; Thanh, N. T. K.; Christopher Doty, R.; Hussain, I.; Nichols, R. J.; Schiffrin, D. J.; Brust, M.; Fernig, D. G. Rational and Combinatorial Design of Peptide Capping Ligands for Gold Nanoparticles. *J. Am. Chem. Soc.* ***2004***. https://doi.org/10.1021/ja0487269.

4. Details of the impact

Understanding chemistry requires an appreciation and understanding of 3D structures and is extremely challenging. Current methods of representing them in textbooks, on blackboards, and paper are inadequate and teaching this material relies on diagrams which are sometimes unconvincing. Our solution was the creation of interactive 3D structures and animated 3D calculated reaction sequences for inspection, all controlled by designed web pages requiring no special software. Users can manipulate the structures in 3D and elect to change the representation to suit their needs using the “Controls”. ChemTube3D has become a crucial platform for University of Liverpool and UK chemistry. It facilitates the training of chemists in leading edge scientific skills, and it utilises open access digital platforms as a highly scalable means to create the widest possible pedagogical impact from our research.

Public engagement with Chemtube3D.com: We chose, in 2008, to make this an Open Educational Resource (OER) to provide free access to our resource for users around the world to maximise the reach and impact of the project. Users can easily find the resource through search engines with Chemtube3D ranked #1 on Google for >200 chemistry related search queries including “chemistry animations”. [5.1] Chemtube3D has rapidly become a leading educational resource with 32000 direct links to individual pages of ChemTube3D from other web sites. **Google Analytics during the REF period** [5.1] **shows that the site received 13.8 million page views with >5 million users. Chemtube3D is being used across the world with users from 190 countries accessing the site**. The USA and India make up ca. 50% of the total traffic, with smaller numbers from UK, Canada, South Korea, and China as well. Users are engaging with the site, accessing on average two pages per session with a duration of >2 minutes demonstrating engagement. Complex structures are typically studied for longer with an average of >5.5 min spent on the peptide-based MOF (ZnCar) structures. Until the recent site redesign, the vast majority of the pages had the option to display a “Larger View” of the structure and this event was tracked independently [5.1]. The Larger view option was the second most popular page on the entire site and a long average view duration confirming that the **users spend time examining and interacting with the animations in detail, improving their learning and understanding**. The redesigned website (Aug 2019) now has much larger dynamically resizing model spaces which has led to an increase in dwell time [5.1].

Demand led to the launch of an iOS (October 2017, rating 4.6*) and Android app (September 2018, rating 4.4*) [5.3] The apps have been installed >18,000 times to date and the popularity of the site has led to a launch of a Facebook community with 5000 members, dominated by residents of the Indian subcontinent, and linked to ChemTube3D providing an opportunity for direct user-to-user interaction on chemical education topics. Based on the success of the mobile apps, user feedback, and the trend towards increasing use of web resources on mobile devices, ChemTube3D was redesigned in 2019 to optimise performance on mobile devices and 42% of the users are now mobile since August 2019.

The originally developed solid-state inorganic structure pages are one of the most popular sections of the site, directly connecting to the sphere-packing derived structure of Cs_3C_{60}. They have been viewed over 1.5 million times. It is therefore clear that the website and app usage data demonstrates the value of Chemtube3D as both an outreach and educational resource and it provides evidence of an extremely high-level of interest and engagement in the material presented.

Impact on the delivery and design of HEI curriculum: Chemtube3D is being used in educational settings across the world and 58% of users are in the target age range (18-24) [5.1] indicating extensive use of the site by undergraduate students to support their learning. University networks accounted for ca. 10% of users, with the top ten Oxford, Cambridge, Liverpool, Irvine, Manchester, Washington, Berkeley, USCD, Durham, and UCLA and correlating to leading large chemistry departments around the world [5.1]. **The interactive structures of Chemtube3D are also used extensively by HEI providers in the delivery of curriculum**. Specialised web site analytics provided by Oribi were run in Nov-Dec 2020 revealing that **>80 University/School virtual learning environments directed their students to ChemTube3D in just a seven-week period** [5.4] providing unambiguous evidence of the educational value of Chemtube3D and that it has become part of the curriculum at other HEI's. A full list of the VLE's from the snapshot is given in evidence 5.4 and includes leading chemistry departments in the UK (Imperial, Cambridge, UCL, Bristol) and abroad (Monash, Waterloo, Moscow State, Grenada). A description of how educators use Chemtube3D to improve attainment is provided by an Associate Professor of Organic Chemistry at the Università di Torino, a University which has linked the site 92 times to course content in their VLE. "*If they comprehend correctly every mechanism step, the verification of their knowledge should be a matter of seconds, giving them the opportunity to self-evaluate their comprehension level of what they studied. This approach, thanks to your animations, granted them at least 2-3 points more on their final score (on a scale of 30 as the top score, as usual for Italian universities), with respect the previous years in which we had no animations to show."* [5.5]. During the COVID-19 pandemic there has been a shift to online-teaching making visualisations of complex structures and mechanisms of even greater value to chemical educators, as described by a Professor at the Federal University of ABC in the state of São Paulo, Brazil "*when remote teaching/learning became a must due to pandemic restrictions, ChemTube3D was a game-changer*" [5.5].

Three leading Oxford University Press textbooks have been updated to integrate the web-based resources of Chemtube3D. The textbooks are (Organic Chemistry (2^{nd} Ed), Chemistry^3, introducing organic, inorganic and physical chemistry (2^{nd} Ed) and Inorganic Chemistry (6^{th} Ed)) they "are adopted at over 40 UK HEIs, and are used more widely than any other chemistry texts in the UK: they command market shares of 89% (Organic), 81% (Chemistry^3) and 75% (Inorganic). These data support the assertion that all three texts have become "*the course companion of choice for a generation of chemistry students*." (>£575k pa sales, [5.6]). **By mapping Chemtube3D assets onto the textbooks, readers are able to migrate between the text and interactive visualisations using 596 bespoke URLs**. The value of Chemtube3D, a research derived resource, to HEI education is described by the Editor in Chief, Natural and Social Sciences of the publisher "*they* [Chemtube3D] *enable users to visualise and actively manipulate both molecular structures and reaction mechanisms featured in our texts in three dimensions. This functionality adds another dimension – quite literally – to the pedagogical value of our texts, taking the user beyond two-dimensional representations of structures and reaction schemes that we are able to present in print*". [5.6] **Chemtube3D is also used extensively within the very popular free to access online LibreTexts Chemistry.** The design of Chemtube3D means pages can be further customised as demonstrated by the use of our animations within 849 different LibreText pages, providing an enhanced learning experience. [5.1]

Impact on the delivery and design Chemistry education at schools: Chemistry animations and interactive models are of particular value to A-level (16-18 age range) students as the curriculum introduces students to the concepts of the shapes of molecules (VSEPR theory), organic reaction mechanisms and the chemistry of polymers. All topics which are hard to address with conventional 2D learning resources. Chemtube3D has a dedicated A-level section covering these key topics, 690k users have interacted with the VSEPR pages alone over the REF period demonstrating their value as an educational resource.[5.1] The resources are accessible by teachers either directly or through links on specialist websites designed to support educators in the 11-19 age range, including notably the Royal Society of Chemistry Education Resources, the Association for Science Education pages, and a-levelchemistry.co.uk.. Analysis of networks using the site also shows substantial levels of traffic being directed from openchem.org, a free to use online homework-quiz system and in the resources of nearpod.com, a specialist company that provides pre-made interactive lessons to US high schools (120 million students engaged with lessons in 2019-2020) demonstrating that Chemtube3D has been embedded within these teaching materials [5.4]. Chemtube3D has now entered the AQA A-level scheme of work [5.7] with teachers being directed to cover 3D representations of organic molecules with the interactive structure and bonding pages of the site being a recommended resource.

The vast number of users of the school-level education resources makes it hard to evidence specific examples of the role of Chemtube3D on the design and delivery of curriculum outside of the UK directly. However, examples of usage patterns of pages provide an illustration of the global role that is playing in the delivery of school level education. In both 2018 and 2019 a cluster of users from the Los Angeles County Office of Education network consulted the sodium chloride structure. The repeat usage of the same pages demonstrates the site has been embedded in the curriculum. Similarly, 169 users from Claremont CA all accessed the Lithium Iron Phosphate page on a single day indicating the use of the site in the local authorities' high school curriculum. Numerous further examples of clustered usage across the UK, USA and India are found within the Google analytics data. The most striking single event occurred on 16-17 June 2019 when 659 users from across India viewed the page dedicated to the symmetry of diborane. The date coincides with the National Chemistry exam in India CSIR-NET demonstrating that these students were all consulting ChemTube3D at the same time for their exam [5.1].

Recognition for ChemTube3D: Chemtube3D and the contribution of Greeves to Chemistry outreach and education has been recognised through the RSC Nyholm Education Prize 2015 for the creation of Chemtube3D [5.8] and by the award of a National Teaching Fellowship with the citation for describing his work as a *"a world leader in developing web-based three dimensional animations to support teaching in organic chemistry - a new tool that really does open up new horizons for both the student and the teacher"* [5.9].

5. Sources to corroborate the impact

5.1 Selected Google Analytics data for ChemTube3D.com 2013-present

5.2 JISC project description and report "Supporting Lifelong Learning: Enhancing the value of interactive 3D chemistry" Last accessed 8/12/20. https://www.webarchive.org.uk/wayback/archive/20140614104945/http://www.jisc.ac.uk/whatwedo/programmes/elearning/ltig/ichem3d.aspx

5.3 a) ChemTube3D on Apple App Store for iOS app https://itunes.apple.com/gb/app/chemtube3d/id1291952162 Last accessed 8/12/20.
b) ChemTube3D on Google Play Store for Android app https://play.google.com/store/apps/details?id=www.chemtube3d.com Last accessed 8/12/20.

5.4 Specialised web site analytics provided by Oribi https://oribi.io/ were run in Nov-Dec 2020

5.5 a) Testimony from an Associate Professors at the Università di Torino
b) UNITO Virtual Learning Environment with direct links to 92 different pages on ChemTube3D http://www.iorgchem.unito.it/index.php/en/ Last accessed 8/12/20
c) Testimony from the Federal University of ABC in the state of São Paulo.

5.6 Letter from Editor in Chief, Natural and Social Sciences, Oxford University Press

5.7 AQA Scheme of work AS Chemistry https://www.aqa.org.uk/subjects/science/as-and-a-level/chemistry-7404-7405/teaching-resources Last accessed 14/1/21

5.8 RSC Nyholm Prize for Education 2015 for the creation and development of ChemTube3D https://edu.rsc.org/news/rsc-2015-education-awards/2000334.article Last accessed 8/12/20.

5.9 National Teaching Fellow award 2009 to Prof Nick Greeves https://www.heacademy.ac.uk/person/dr-nick-greeves Last accessed 8/12/20.