



Publishing science in a 21st century style

Webinar Series



Matteo Cavalleri and Alberto Pepe

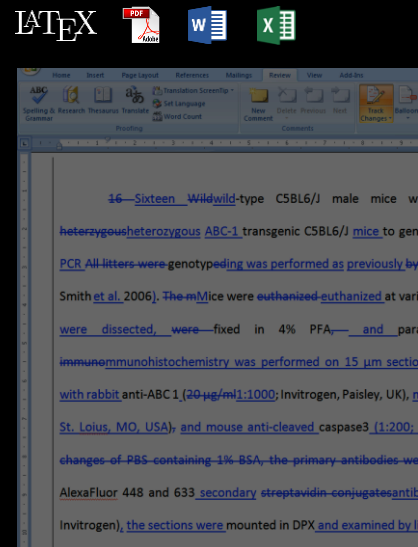
ATYPON WILEY

Researchers produce
21st century research



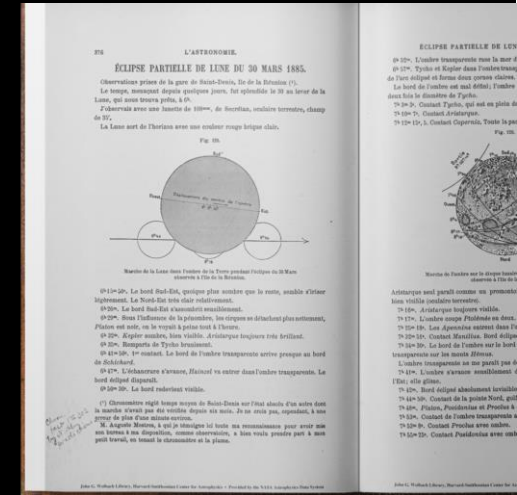
Research is becoming more
computational, collaborative, data-driven, automated, and web-based.

Written up using
20th century technology



Most paper formats are not natively
collaborative, data-driven, version controlled, or backwards compatible.

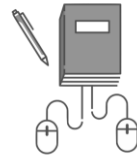
Published in a
17th century format



A centuries-old research “paper” is
much like papers we publish, share
and read today (i.e., **static, 2D PDFs**)

THE CHALLENGE

Current publishing workflows “flatten” rich research content



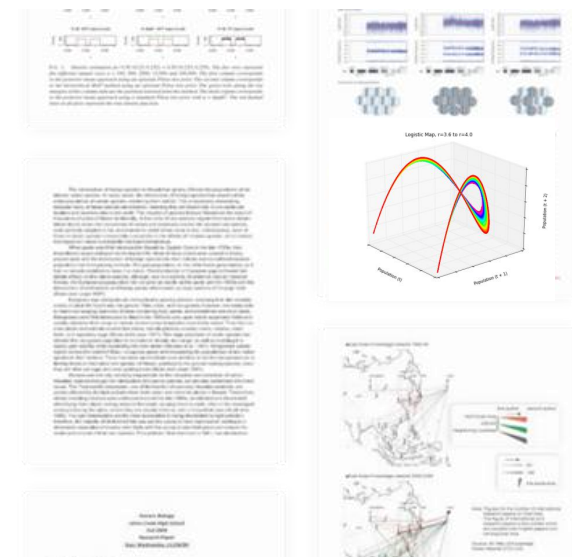
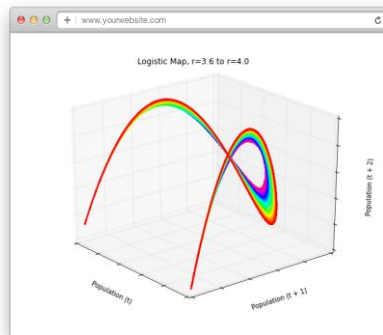
**AUTHORING
TOOLS**



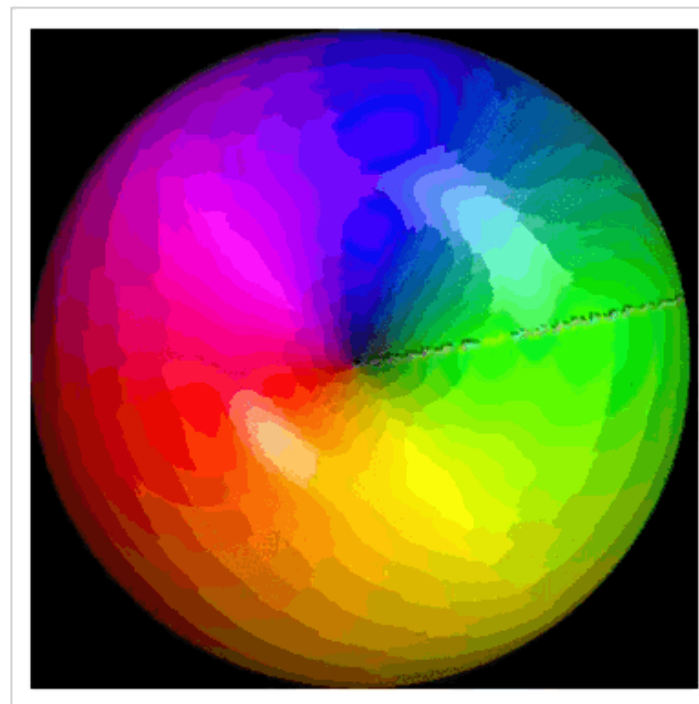
**PEER REVIEW
SYSTEMS**



**PRODUCTION &
TYPESETTING**



Now, the *time-dependent* (TD) version of our orbital, $e^{-iEt}\psi_+$, has a *rotating* phase factor. If multiplication by a phase factor rotates an angular momentum eigenfunction, then a continually changing phase factor will cause such a wavefunction to spin round and round (a feature of orbital angular momentum functions noted in Ref. 10). This is shown in Animation 1A. Now, this necessarily causes both the real and imaginary components—which look like *p*-orbitals – to spin around as well. This is shown in Animation 1B, which depicts $\text{Re}[e^{-iEt}\psi_+]$ (the imaginary component, $\text{Im}[e^{-iEt}\psi_+]$, looks the same as $\text{Re}[e^{-iEt}\psi_+]$ but rotated $\pi/2$ anticlockwise, so is not plotted. t is in arbitrary units with E dropped for simplicity).

**Animation 1A**
[Open in figure viewer](#) | [PowerPoint](#)

 Time-dependent p_+ -orbital ($e^{-iEt}\psi_+$), phase-colored.
Metrics

Citations: 2

**Details**

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**Research Funding**

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Keywords

molecular orbitals

spin-orbit coupling

visualization

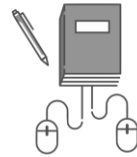
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11 May 2018

THE CHALLENGE

Current publishing workflows “flatten” rich research content



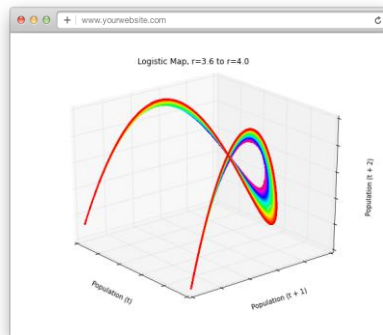
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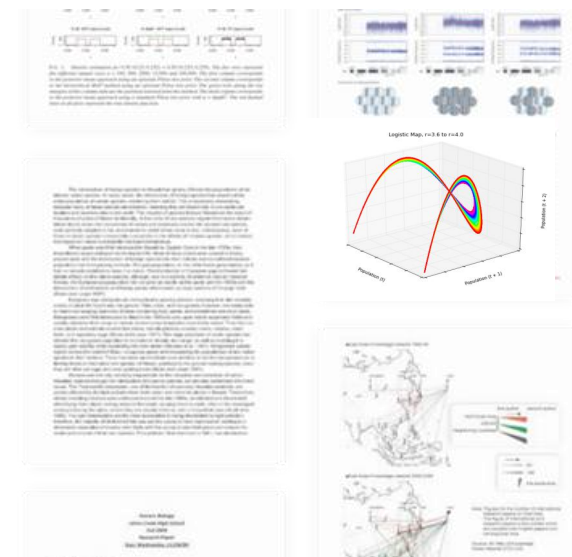
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PRODUCTION &
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Can preprints
bridge this gap?



preprint

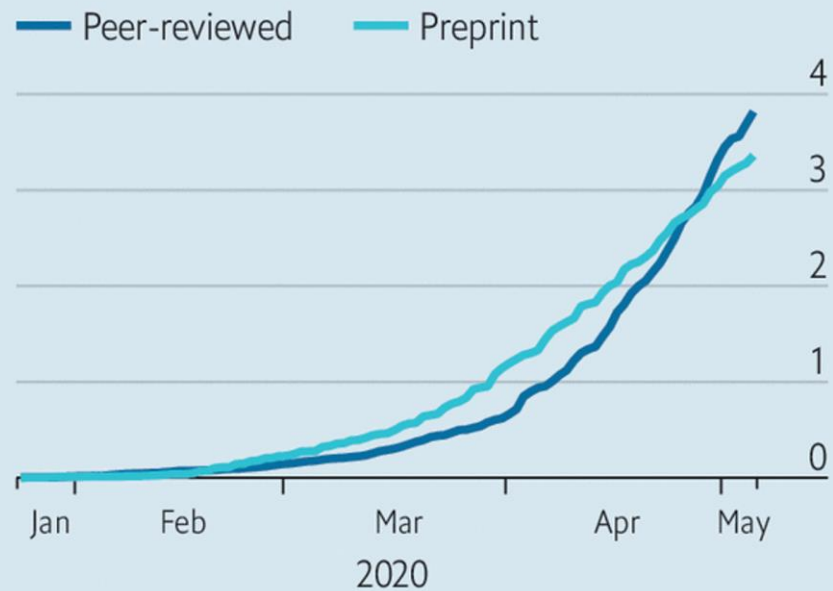
Preprint |'prē-,print|

noun

- 1.** An early research output.
- 2.** A version of a scholarly paper that precedes formal peer review and publication in a peer-reviewed journal. The preprint, often a non-typeset version available free, persists after a paper is published in a journal.

Quick studies

Research papers concerning covid-19, total, '000
To May 5th



Source: Primer

The Economist

Before 2020, preprints were few and limited to the physical sciences

In 2020, for each peer reviewed publication about COVID-19, a preprint was posted

In total, 30,000 preprints about COVID-19 appeared in 2020. A third of them were mentioned by news articles (cf w 1% baseline)



Allergy

EUROPEAN JOURNAL OF ALLERGY
AND CLINICAL IMMUNOLOGY



LATEST ISSUE >

Volume 76, Issue 12
December 2021

Edited By: Cezmi Akdis

Impact factor: 13.146

2020 Journal Citation Reports (Clarivate Analytics): 1/28 (Allergy) 9/162 (Immunology)

Online ISSN: 1398-9995

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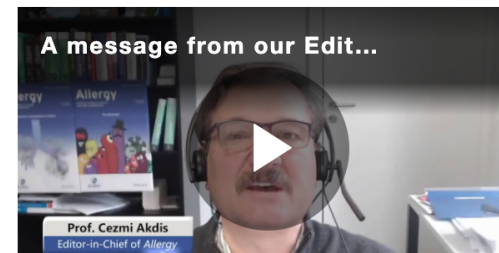
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Prof. Cezmi Akdis
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Management and outcome of suspected and confirmed COVID-19 (SARS-CoV-2) vaccine hypersensitivity.

ANAPHYLAXIS COVID-19 SARS-COV VACCINES

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1,238 VIEWS

9 0 10 0

Allergenic components of the mRNA-1273 vaccine for COVID-19: possible involvement of polyethylene glycol and IgG-mediated complement activation

COVID COVID-19 SARS-COV VACCINES

L¹ N¹ B¹ C¹ +3 Ludger Klimek, Natalija Novak, Beatriz Cabanillas , Marek Jutel, Jean Bousquet

Abstract

Following the emergency use authorization of the vaccine mRNA-1273 on 18th December 2020 in the US and the vaccine BNT162b2 one week earlier, two mRNA vaccines are in currently used for the prevention of coronavirus disease 2019 (COVID-19). Phase 3 pivotal trials on both vaccines excluded individuals with a history of allergy to vaccine components...

Peer review status: **PUBLISHED**30 Dec 2020 Submitted to *Allergy* [Show details](#)Nov 2021 Published in *Allergy* volume 76 issue 11 on pages 3307-3313. [10.1111/all.14794](https://doi.org/10.1111/all.14794)

Cite as: Ludger Klimek, Natalija Novak, Beatriz Cabanillas, et al. Allergenic components of the mRNA-1273 vaccine for COVID-19: possible involvement of polyethylene glycol and IgG-mediated complement activation. *Authorea*. January 01, 2021.

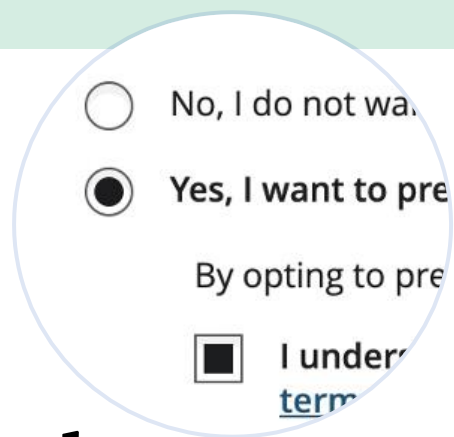
DOI: [10.22541/au.160952242.21038379/v1](https://doi.org/10.22541/au.160952242.21038379/v1)



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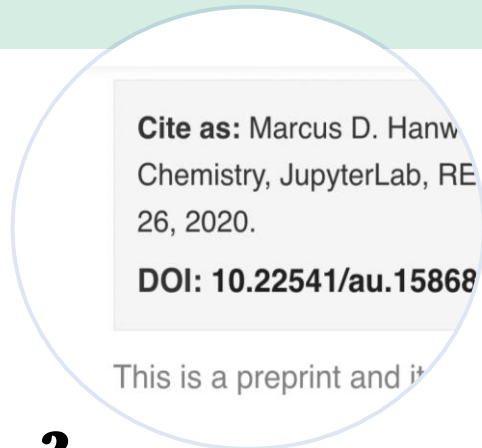
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1

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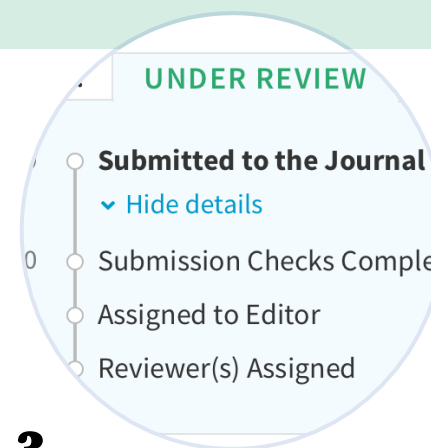
Cite as: Marcus D. Hanwell, *Journal of Chemical Education*, 2020, 97(12), 26, 2020.

DOI: [10.22541/au.15868](https://doi.org/10.22541/au.15868)

This is a preprint and it has not been certified by peer review.

2

When manuscript is sent to reviewers, it is ingested and posted with DOI



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Submitted to the Journal

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0 Submitted to *Journal of the American Chemical Society*

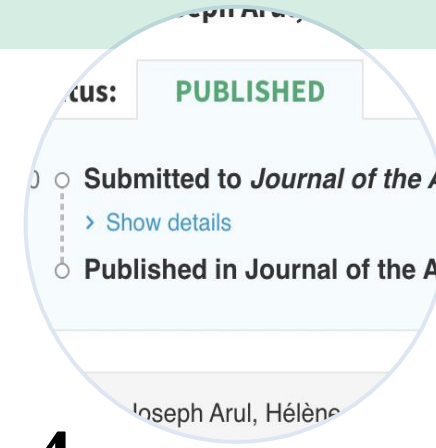
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Assigned to Editor

Reviewer(s) Assigned

3

Status automatically updated as manuscript goes through review



PUBLISHED

Submitted to the Journal

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0 Submitted to *Journal of the American Chemical Society*

Published in *Journal of the American Chemical Society*

Joseph Arul, Hélène

4

Paper published, automatic link to Version of Record assigned

45 participating journals

In 2020: **11K** preprints were posted via
Under Review (**1.5k** about COVID-19)

Health Sciences

Allergy
International Journal of Obstetrics and Gynecology
British Journal of Clinical Pharmacology
British Journal of Pharmacology
Clinical Case Reports
Clinical Otolaryngology
Computational and Systems Oncology
Echocardiography
Influenza and other respiratory viruses
International Journal of Clinical Practice
Journal of Cardiac Surgery
Journal of Cardiovascular Electrophysiology
Journal of Evaluation in Clinical Practice
Pediatric Allergy and Immunology
Pediatric Blood & Cancer
Pediatric Pulmonology
Transboundary and Emerging Diseases

Life Sciences

Advanced Genetics
Biotechnology Journal
Biotechnology and Bioengineering
Clinical & Experimental Immunology
Ecology and Evolution
Ecology Letters
Human Mutation
Hydrological Processes
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Physical Sciences

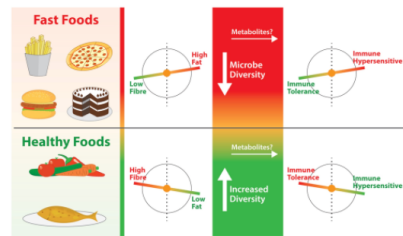
AIChE Journal
Applied AI Letters
Engineering Reports
Fatigue & Fracture of Engineering
International Journal of Quantum Chemistry
Journal of the American Oil Chemists' Society
Materials & Structures
Mathematical Methods in the Applied Sciences
Natural Sciences
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PUBLIC DOCUMENTS (154) **UNDER REVIEW (35)** STATISTICS MEMBERS SETTINGS

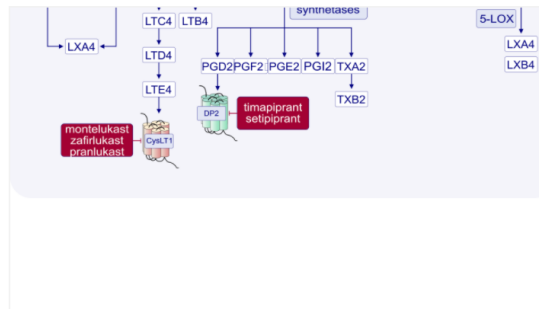
Figure 1. Fiber, fat and the microbiome



Role of Dietary Fiber in Promoting Immune Health -- An EAACI Position Paper

Carina Venter and 21 more
November 28, 2021

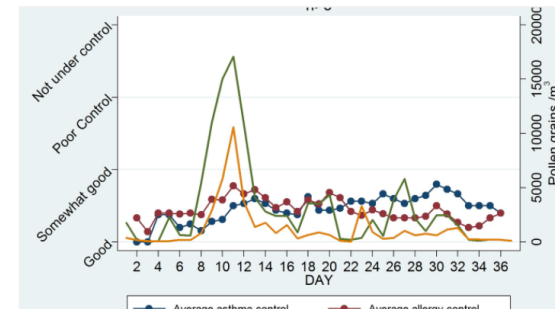
Microbial metabolism of specific dietary components, such as fiber, contribute to the



Effects of non-steroidal anti-inflammatory drugs and other eicosanoid pathway modifie...

Milena Sokolowska and 16 more
November 26, 2021

Non-steroidal anti-inflammatory drugs (NSAIDs) and other eicosanoid pathway modifiers are



Exposure to birch pollen and the risk of allergic and asthmatic manifestations

Timo Hugg and 4 more
November 24, 2021

This is a Letter and does not include an abstract.



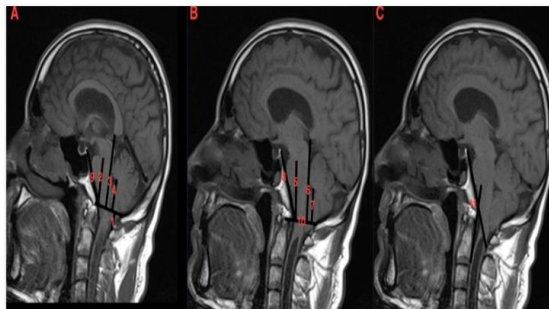
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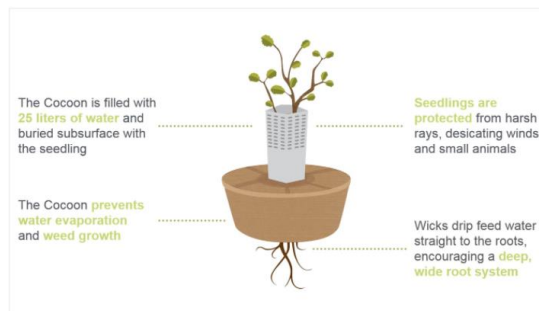
UNDER REVIEW (2133)



Multi-parameter-based Radiological Diagnosis of Chiari Malformation using Machine Lea...

BT **DD** Bora Tetik and 7 more
April 19, 2021

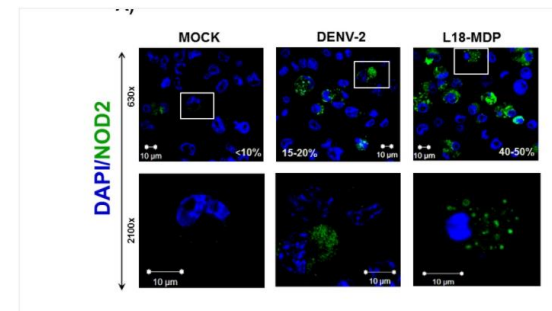
Background: The known primary radiological diagnosis of Chiari Malformation-I (CM-I) is



Water-saving techniques for restoring desertified lands: some lessons from the field

VC **A** Vicenç Carabassa and 15 more
April 19, 2021

In the light of the current climate crisis, one of the most serious ecological threats is the



Dengue virus type 2 replication is limited by activation of NOD2 and its interactions...

DD **A** Diana Domínguez-Martínez and 5 more
April 19, 2021

The nucleotide-binding domain (NBD) and leucine-rich repeat receptors, such as NOD-like





Scott P. Egan @scottpegan Jul 14

New preprint!: Tissue-specific gene expression shows [#cynipid](#) [#wasps](#) repurpose host gene networks to create complex & novel parasite-specific organs on [#oaks](#).

Led by Dr. Ellen Martinson (@[wasp_venom](#)); in collaboration w/ Dr. Jack Warren & me. More to come.

doi.org/10.22541/au.15...

1 5 24



Emma Moffett @EmmaMoffett1 Oct 10

Multigenerational exposure to warm temperatures reduces metabolic rate but increases boldness! Check out our new preprint at [@authorea](#) [#paceoflife](#) [#thermaladaptation](#) [@KevinSimoNZ](#) [@davefryx](#) doi.org/10.22541/au.16...

1 4 11



Micah Brush @MicahBrush 2d

New preprint is up!

authorea.com/users/344416/a...

This analysis was mostly done by an undergraduate in our group, Juliette Franzman, with data collected at RMBL over many years by [@benjaminblonder](#) and his graduate student Courtenay Ray.

1 2 5



David M Watson @DOCTOR... Nov 25

My first preprint, led by Robert Nespolo and Francisco Fonturbel. The ecology and evolution of the Monito del monte, a relict species from the southern South America temperate forests. Let us know what you think...

authorea.com/users/265191/a...

6 1 16



Timothy P. Cripe @KidsOnc... May 7

[@nationwidekids](#) leads discussion with a new record - 7 days from concept to acceptance and posting on public server! Pediatric Cancer Research: Surviving COVID-19 authorea.com/users/319136/a...

2 5



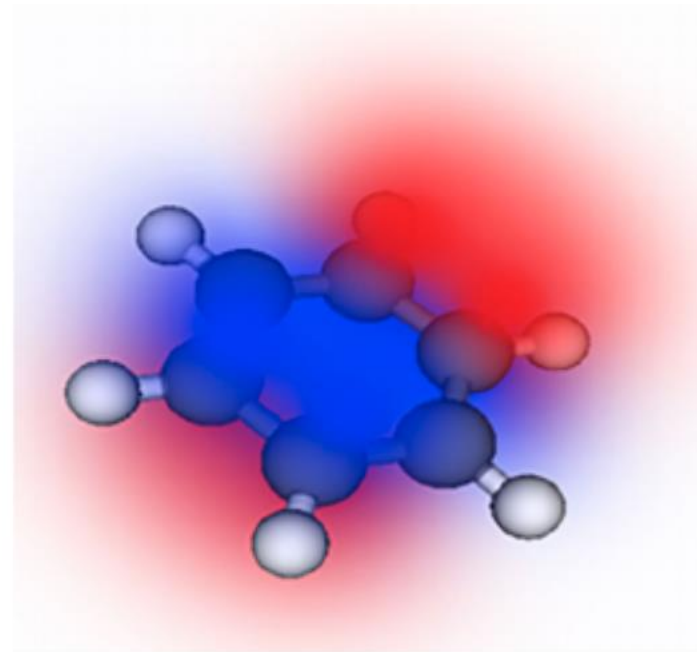
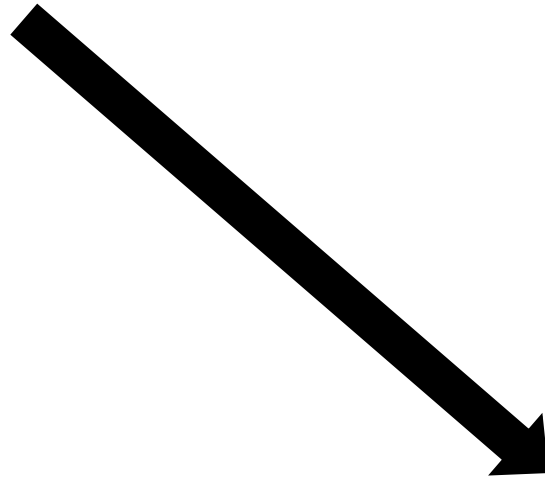
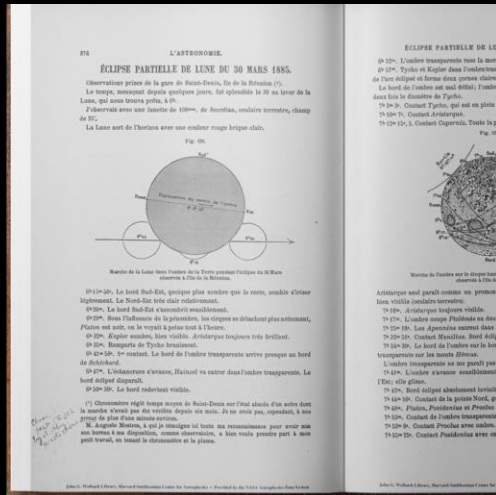
Heidi Schutz @heidihabilis 6d

So pleased to share a preprint of our recently submitted paper. Cheers to an amazing group of co-authors [@PhysIsPhun](#) [@pumtiwitt](#) [@WrightingApril](#) [@kateboersma](#) [@stephshep](#) Lathiena Manning [@MalischPhd](#) & Roni Ellington authorea.com/users/343274/a...

5 35 67

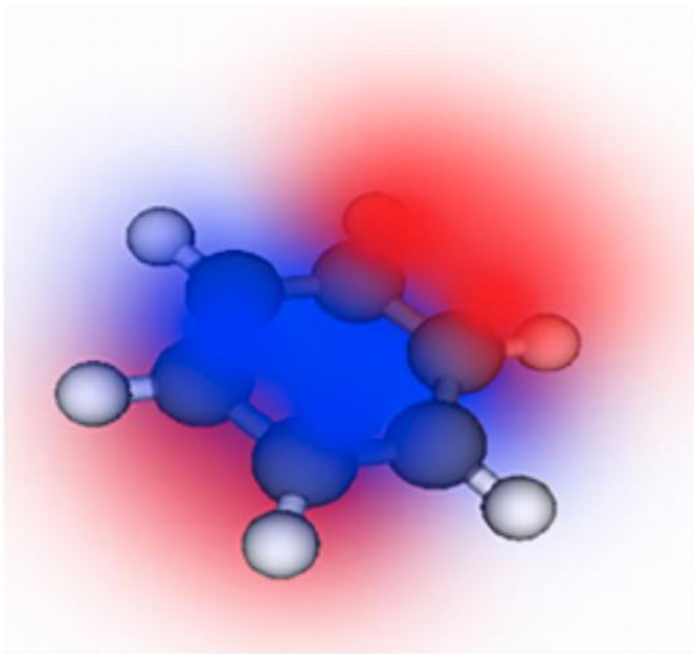
Researchers produce
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Published in a
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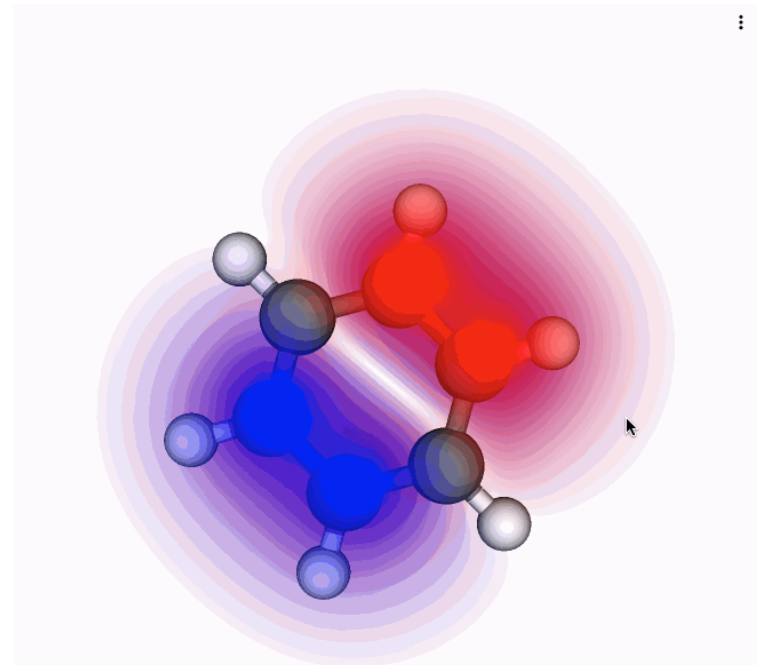


What's wrong with that?

Figure 1. An H α (+ continuum) image of M16, obtained with the CTIO/Michigan Curtis Schmidt. The stars responsible for exciting the nebula are ~ 2 pc from the elephant trunks, in the top right quadrant of the image. Approximate locations of the fields imaged with UNSWIRF (1.6 arcmin in diameter) are indicated. North is up and east is to the left.



Data in articles lack depth...



...and they lack breadth...

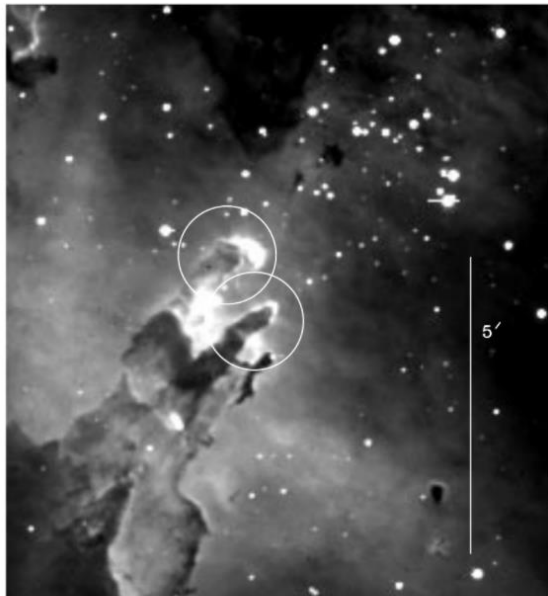
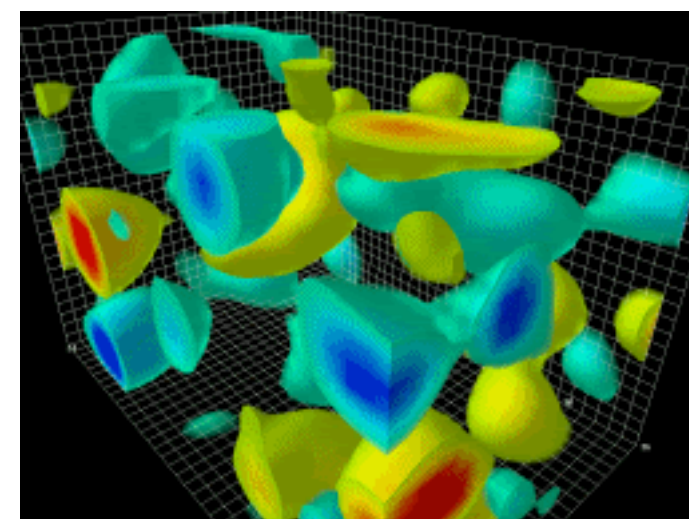
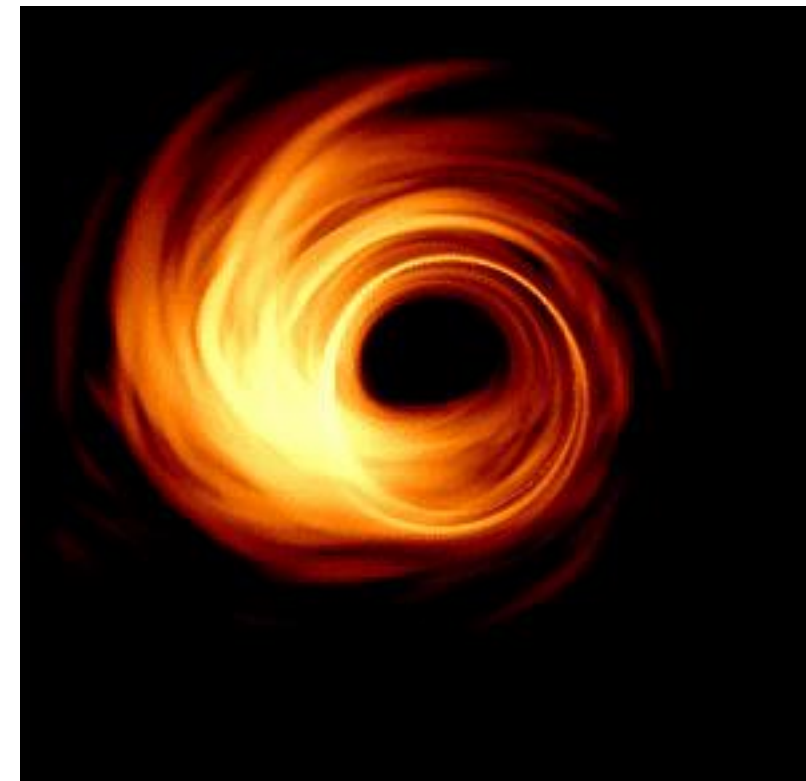
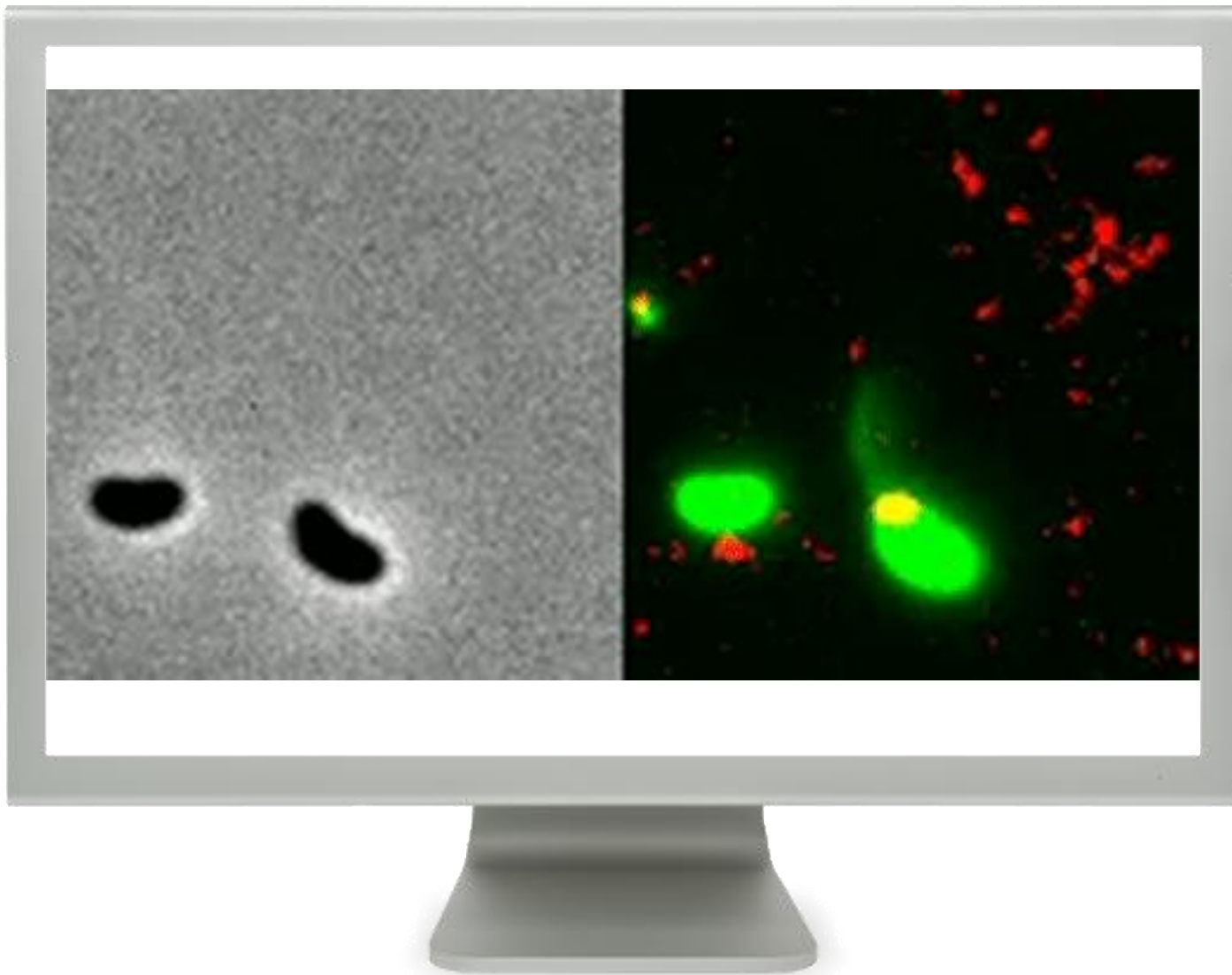


Figure 1. An H α (+ continuum) image of M16, obtained with the CTIO/Michigan Curtis Schmidt. The stars responsible for exciting the nebula are ~ 2 pc from the elephant trunks, in the top right quadrant of the image. Approximate locations of the fields imaged with UNSWIRF (1.6 arcmin in diameter) are indicated. North is up and east is to the left.



AAS World Wide Telescope



Researchers analyze data interactively in the lab, it takes work for them to make them static and dumb for a article publication

Supplementary Information
are where data go to die

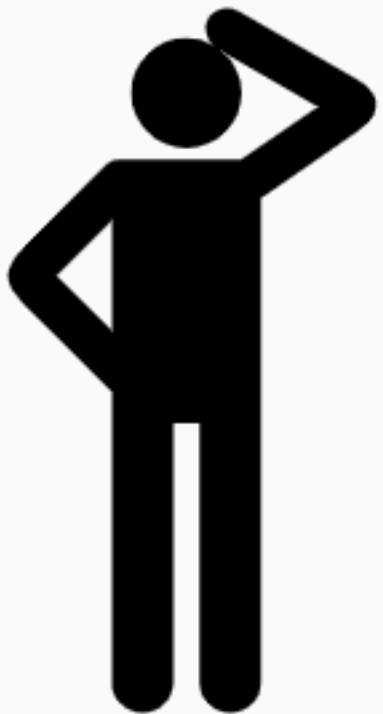
Furthermore, as we already highlighted above, the main text is often not well integrated with the supporting information provided in supplementary material. Readers often have to sift through tens or hundreds of pages of text to find information simply referenced from the main text as 'see Supplementary material'.

Use and mis-use of supplementary material in science publications

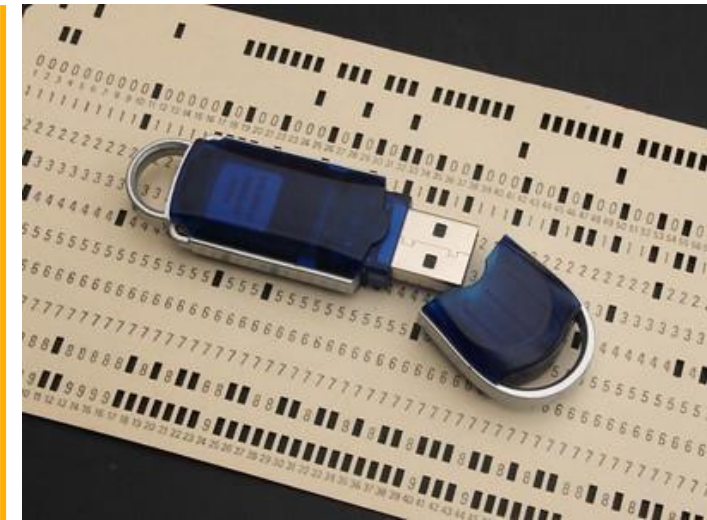
Mihai Pop & Steven L. Salzberg

BMC Bioinformatics 16, Article number: 237 (2015) | [Cite this article](#)

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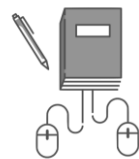
Where is the code? Does it
even work in my computer?



...while data and code may be available in repositories external to the corresponding article, it takes readers and reviewers considerable effort to verify the software and re-run analyses with, say, changed parameters. [10.22541/au.160211021.13787691/v1](https://doi.org/10.22541/au.160211021.13787691/v1)



WELCOME
TO THE
FUTURE



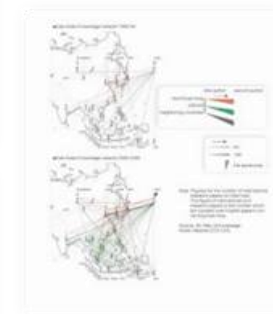
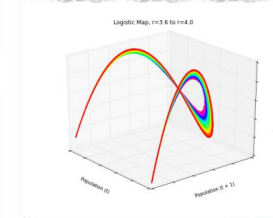
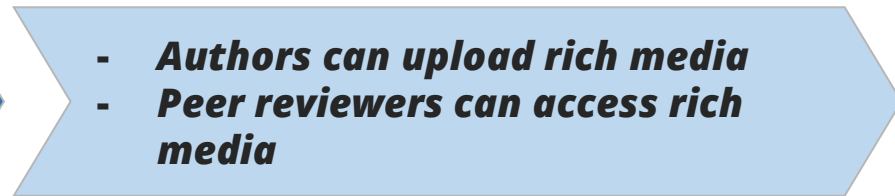
AUTHORING TOOLS



PEER REVIEW SYSTEMS



PRODUCTION & TYPESETTING











Author has options to **edit** preprint and publish new versions

The screenshot shows the Authorea interface for a preprint. At the top, the 'AUTHOREA' logo is on the left, and 'EDIT' and 'PUBLISH' buttons are on the right. A 'DOWNLOAD PDF' button is visible below the logo. The title of the preprint is 'Open Chemistry, JupyterLab, REST, and Quantum Chemistry'. Below the title, the authors are listed: Marcus D. Hanwell, Chris Harris, Alessandro Genova, Mojtaba H, Muammar El Khatib, Patrick Avery, Johannes Hachmann, and Wibe. A dropdown menu is open, showing options: 'Manage collaborators', 'Share via link', 'Share with a group', 'Submit to a collection', 'Submit to a journal', and 'View all options'. The abstract section contains the text: 'Quantum chemistry must evolve if it wants to fully leverage the benefits of the internet age, where the world wide web offers a vast tapestry of tools that enable users to communicate and interact with complex data at the speed and convenience of a button press. The Open Chemistry project has developed an open source framework that offers an end-to-end solution for producing, sharing, and visualizing quantum chemical data interactively on the web using an array of modern tools and approaches. These tools build on some of the best open source community projects such as Jupyter for interactive online notebooks, coupled with 3D ...'. The peer review status is 'PUBLISHED'. A timeline shows two events: '08 Apr 2020 Submitted to IJQC Special Issue' and '17 Sep 2020 Published in International Journal of Quantum Chemistry. 10.1002/qua.26472'. The citation information is: 'Cite as: Marcus D. Hanwell, Chris Harris, Alessandro Genova, et al. Open Chemistry, JupyterLab, REST, and Quantum Chemistry. Authorea. August 26, 2020. DOI: 10.22541/au.158687268.81852407/v2'. A version selector shows 'v2 - August 26, 20'. The footer indicates 'Version of Record available at: 10.1002/qua.26472'.

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Open Chemistry, JupyterLab, REST, and Quantum Chemistry

Marcus D. Hanwell , Chris Harris , Alessandro Genova , Mojtaba H , Muammar El Khatib , Patrick Avery , Johannes Hachmann , Wibe 

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Submit to a collection
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Abstract

Quantum chemistry must evolve if it wants to fully leverage the benefits of the internet age, where the world wide web offers a vast tapestry of tools that enable users to communicate and interact with complex data at the speed and convenience of a button press. The Open Chemistry project has developed an open source framework that offers an end-to-end solution for producing, sharing, and visualizing quantum chemical data interactively on the web using an array of modern tools and approaches. These tools build on some of the best open source community projects such as Jupyter for interactive online notebooks, coupled with 3D ...

Peer review status: PUBLISHED

08 Apr 2020 Submitted to *IJQC Special Issue* [↗](#)
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17 Sep 2020 Published in *International Journal of Quantum Chemistry*. [10.1002/qua.26472](https://doi.org/10.1002/qua.26472) [↗](#)

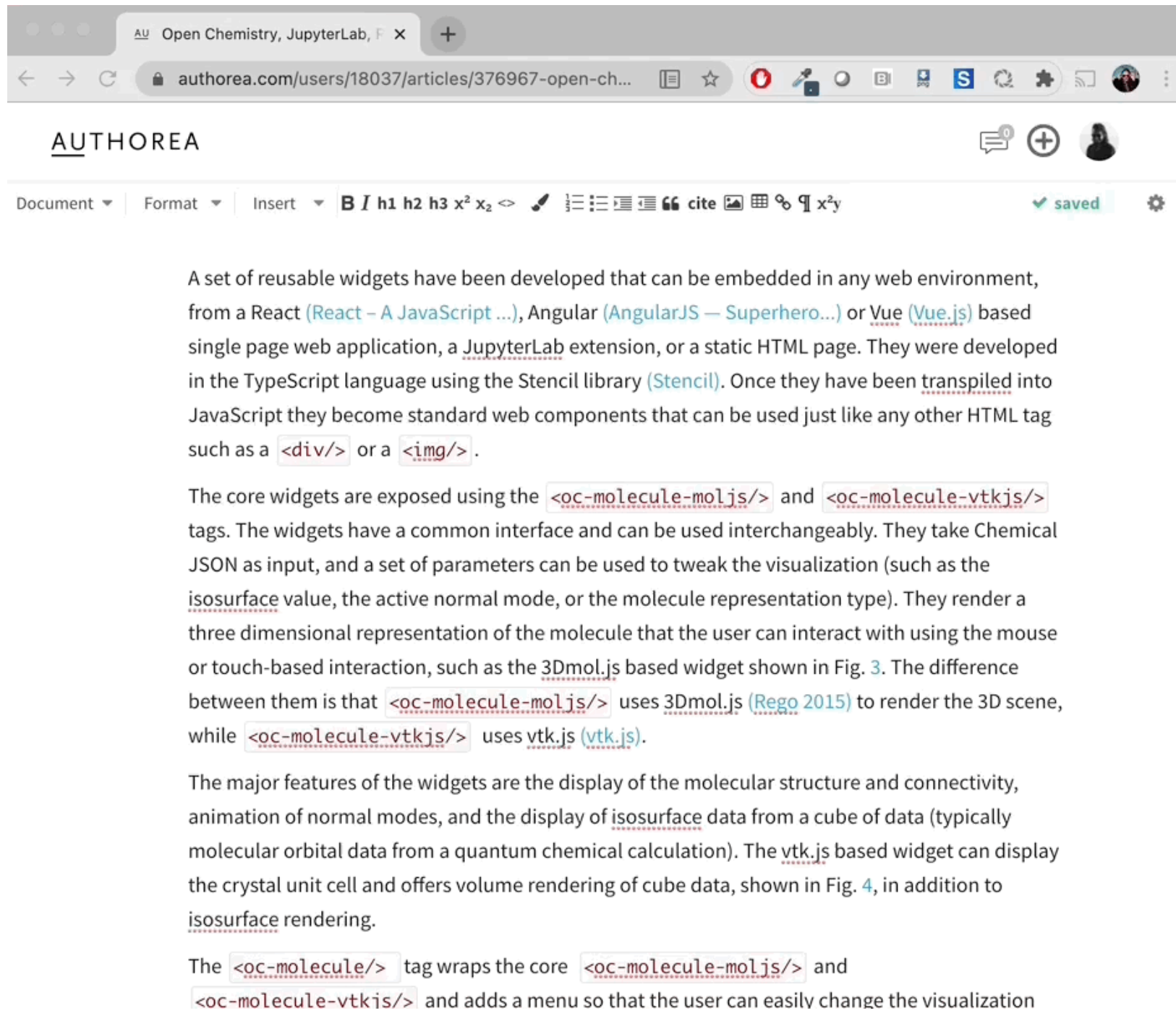
Cite as: Marcus D. Hanwell, Chris Harris, Alessandro Genova, et al. Open Chemistry, JupyterLab, REST, and Quantum Chemistry. *Authorea*. August 26, 2020.

DOI: [10.22541/au.158687268.81852407/v2](https://doi.org/10.22541/au.158687268.81852407/v2)

v2 - August 26, 20

Version of Record available at: [10.1002/qua.26472](https://doi.org/10.1002/qua.26472)

In edit mode, author can add **data, code, Jupyter notebooks**, and replace static figures with **interactive figures**



The screenshot shows the Authorea web editor interface. At the top, there is a browser address bar with the URL `authorea.com/users/18037/articles/376967-open-ch...`. Below the browser, the Authorea logo is visible on the left, and a user profile icon with a plus sign and a notification bell is on the right. A toolbar contains various editing tools such as bold, italic, text size, link, and code blocks. The main content area displays a paragraph of text with several code snippets highlighted in red boxes, including `<div/>`, ``, `<oc-molecule-moljs/>`, and `<oc-molecule-vtkjs/>`. The text describes reusable widgets for embedding in web environments and their use in rendering 3D molecular structures.

AUTHOREA

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A set of reusable widgets have been developed that can be embedded in any web environment, from a React ([React – A JavaScript ...](#)), Angular ([AngularJS – Superhero...](#)) or Vue ([Vue.js](#)) based single page web application, a [JupyterLab](#) extension, or a static HTML page. They were developed in the TypeScript language using the Stencil library ([Stencil](#)). Once they have been [transpiled](#) into JavaScript they become standard web components that can be used just like any other HTML tag such as a `<div/>` or a ``.

The core widgets are exposed using the `<oc-molecule-moljs/>` and `<oc-molecule-vtkjs/>` tags. The widgets have a common interface and can be used interchangeably. They take Chemical JSON as input, and a set of parameters can be used to tweak the visualization (such as the [isosurface](#) value, the active normal mode, or the molecule representation type). They render a three dimensional representation of the molecule that the user can interact with using the mouse or touch-based interaction, such as the [3Dmol.js](#) based widget shown in Fig. 3. The difference between them is that `<oc-molecule-moljs/>` uses [3Dmol.js](#) ([Rego 2015](#)) to render the 3D scene, while `<oc-molecule-vtkjs/>` uses [vtk.js](#) ([vtk.js](#)).

The major features of the widgets are the display of the molecular structure and connectivity, animation of normal modes, and the display of [isosurface](#) data from a cube of data (typically molecular orbital data from a quantum chemical calculation). The [vtk.js](#) based widget can display the crystal unit cell and offers volume rendering of cube data, shown in Fig. 4, in addition to [isosurface](#) rendering.

The `<oc-molecule/>` tag wraps the core `<oc-molecule-moljs/>` and `<oc-molecule-vtkjs/>` and adds a menu so that the user can easily change the visualization

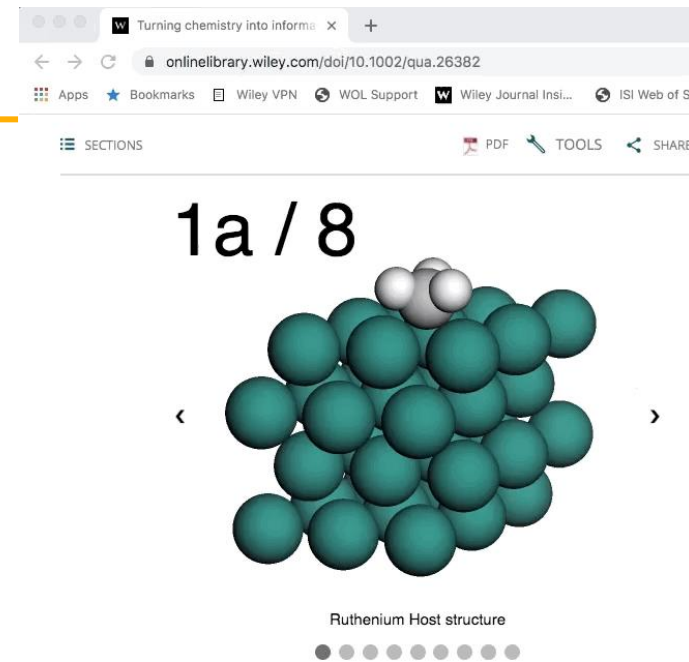
All rich media objects (data, code, notebooks, and interactive visualizations) are pushed and published in the **Version of Record**

The screenshot shows a web browser window with two tabs. The active tab is titled 'Open Chemistry, JupyterLab, REST, and quantum chemistry'. The address bar shows the URL 'onlinelibrary.wiley.com/doi/10.1002/qua.26472'. The page header includes the Wiley Online Library logo and a search icon. The main content area displays the journal title 'International Journal of Quantum Chemistry / Volume 121, Issue 1', the article type 'FULL PAPER', and 'Open Access' status. The article title is 'Open Chemistry, JupyterLab, REST, and quantum chemistry'. The authors listed are Marcus D. Hanwell, Chris Harris, Alessandro Genova, Mojtaba Haghightalari, Muammar El Khatib, Patrick Avery, Johannes Hachmann, and Wibe Albert de Jong. The publication date is 'First published: 17 September 2020' and the DOI is 'https://doi.org/10.1002/qua.26472'. A 'Funding information' section lists several grants from the National Science Foundation and the New York State Center of Excellence in Materials Informatics. At the bottom of the page, there is a dark blue navigation bar with 'About' and 'Sections' links, and a light green callout box stating: 'The HTML version of this article is enhanced with interactive figures, integrated source data, and links to executable code.'

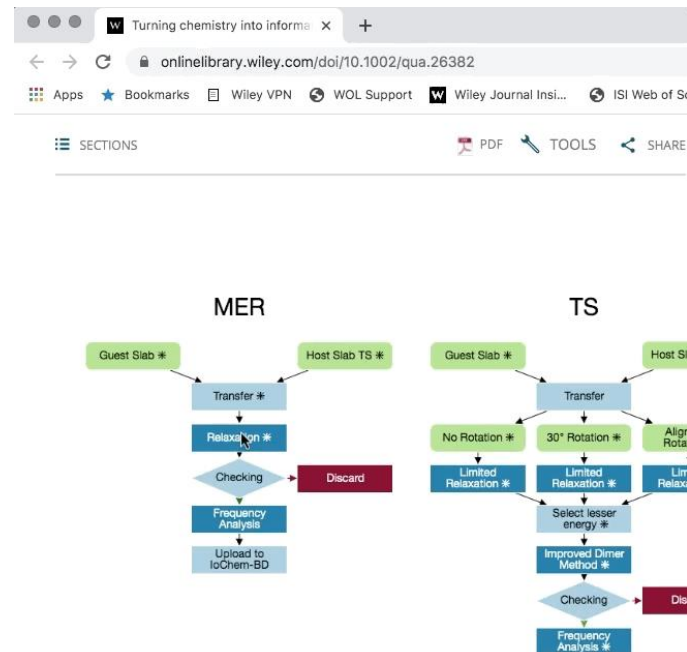
Abstract

Quantum chemistry must evolve if it wants to fully leverage the benefits of the internet age, where the worldwide web offers a vast tapestry of tools that enable users to communicate and interact with complex data at the speed and convenience of a button press. The Open

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All rich media objects (data, code, notebooks, and **interactive visualizations**) are pushed and published in the version of records



~~Supplementary Information are where data go to die~~
Data are connected to the figure that describe them. They are discoverable, indexable, citable, and **usable**



Having trouble viewing this interactive figure? [View static figure](#)



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~~Where is the code? Does it even work in my computer?~~

The code is in the figure, in an executable time capsule

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extended to support execution without a data server and packaged using pip so that it can be installed via the mechanism offered by the Binder project. A blog post was written in December, 2018, describing the approach^[58] and showing the Binder repository with example links to data for calculations^[59] (Figure 6).

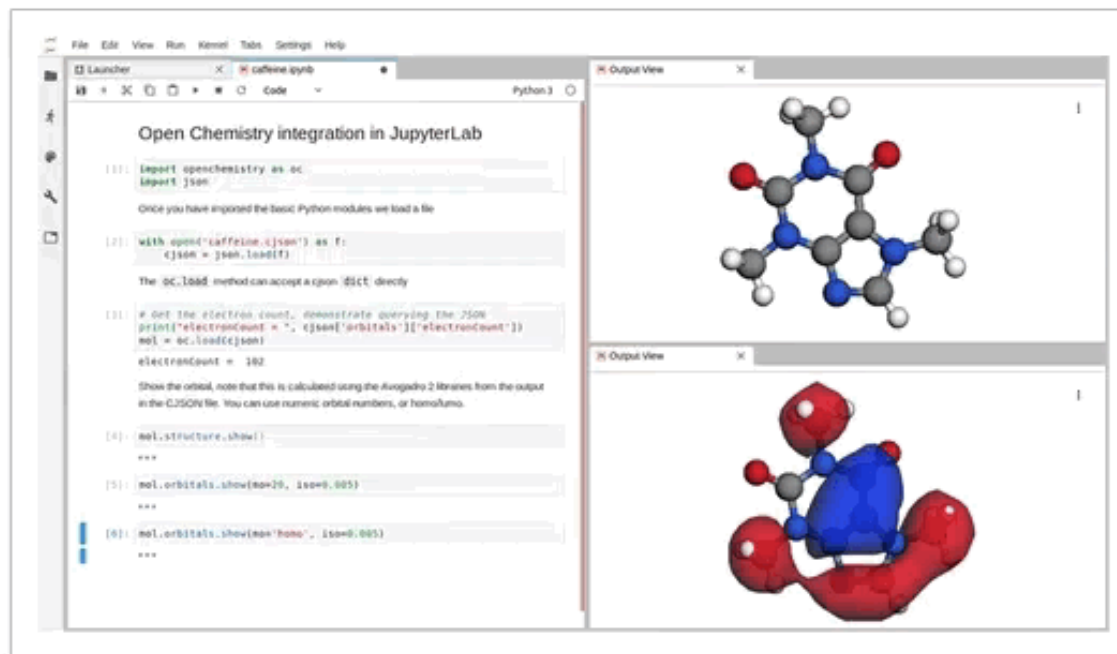


FIGURE 6

[Code](#) | [PowerPoint](#)

The JupyterLab extension allows the visualization of molecular structures in a notebook, with Binder used here to offer a static repository to offer a more interactive exploration of data

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Open Chemistry, JupyterLab, REST, and Quantum Chemistry



Marcus D. Hanwell , Chris Harris , Alessandro Genova , Mojtaba Haghightlari , Muammar El Khatib , Patrick Avery , Johannes Hachmann , Wibe Albert de Jong

Peer Review Material

Review for: "Open Chemistry, JupyterLab, REST, and Quantum Chemistry"

[Anonymous IJQC Reviewer](#)

April 11, 2020

Review for: "Open Chemistry, JupyterLab, REST, and Quantum Chemistry"

[Roberto Di Remigio](#)

May 20, 2020



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Review for: "Open Chemistry, JupyterLab, REST, and Quantum Chemistry"

 Roberto Di Remigio 

Abstract

The manuscript describes the features of a platform developed by the OpenChemistry consortium that bridges many prominent technologies in data sharing, analysis, and visualization. The platform unifies a web-based GUI with few computational backends and can be used to visualize and analyze pre-existing data or newly produced computational results.

The development of this platform is timely and the description in the manuscript is clear and compelling. I recommend the paper be **published with minor revisions**, suggested in the following.

I hereby give permission to publicly associate my name to this referee report.

Editor's Note: *Accepted version of this*

manuscript <https://doi.org/10.22541/au.158687268.81852407/v2>

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1 Referee Report

I would first like to thank the authors for describing their work in a language approachable also to those that are not steeped into novel web-based technologies. The submission is timely and is extremely well-suited for publication in an interactive format. Finally, I couldn't agree more with

Peer review reports,
author rebuttals and
editor notes get **a DOI**
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