Part of SPRINGER NATURE

Publishing data & software

Iulia Georgescu

nature research

Determination of the speed of light

Ole Rømer (1644–1710)

JOURNAL

234

ne seconde de temps.

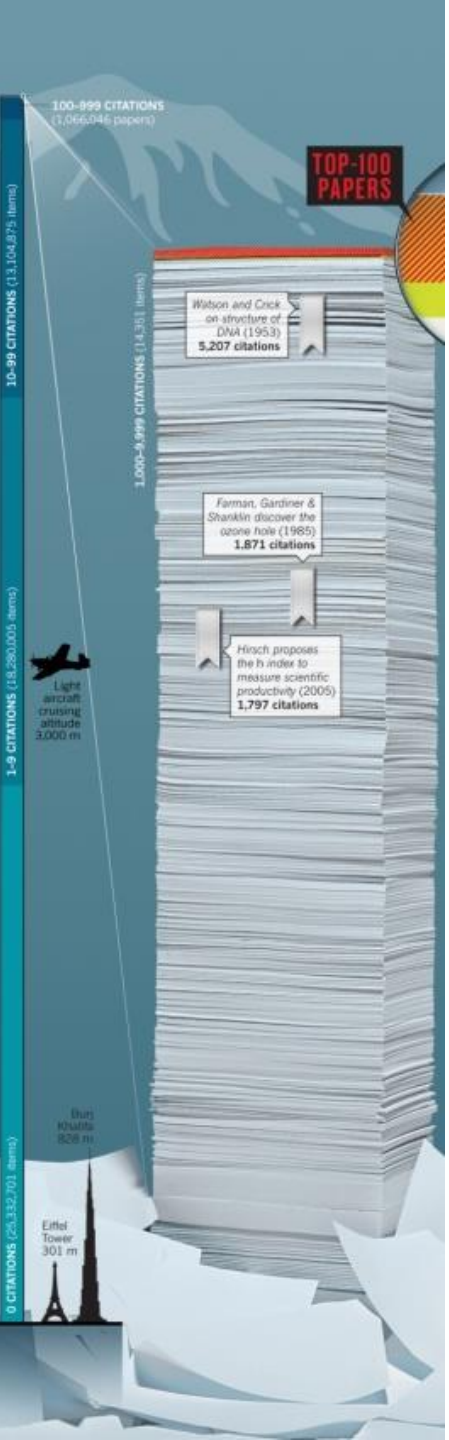
Soit A le Soleil, B Jupiter, C le premier Satellite qui entre dans l'ombre de Jupiter pour en sortir en D, & soit EFGHKL la Terre placée à diverses distances de Jupiter.

Or supposé que la terre estant en L vers la seconde Quadrature de Jupiter, ait veu le premier Satellite, lors de son émersion ou sortie de l'ombre en D; & qu'en suite environ 42. heures & demie après, sçavoir aprés une revolution de ce Satellite, la terre se trouvant en K, le voye de retour en D: Il est manifeste que si la lumiere demande du temps pour traverser l'intervalle LK, le Satellite sera veu plus tard de retour en D, qu'il n'auroit esté si la terre estoit demeurée en K, de sorte que la revolution de ce Satellite, ainsi observée par les Emersions, sera retardée d'autant de temps que la lumiere en aura employé à passer de L en K, & qu'au contraire dans l'autre Quadrature FG, où la terre en s'approchant, va au devant de la lumiere, les revolutions des Immersions paroistront autant accourcies, que celles des Emersions avoient paru alongées. Et parce qu'en 42 heures & demy, que le Satellite employe à peu prés à faire chaque revolution, la distance entre la Terre & Iupiter dans l'un & l'autre Quadrature varie tout au moins de 210. diametres de la

Data

Story: 1676 *Journal des sçavans*

esearch



350 years of scientific publishing

1665

Philosophical Transactions of the Royal Society and *Journal des sçavans* (1665-1792)

2015

>14,000 ISI journals

~58 million papers in Web of Science

nature research

Jim Gray *The Fourth Paradigm*

- **Empirical** (describing natural phenomena)
- **Theoretical** (using models, generalizations)
- **Computational** (simulating complex phenomena)
- **Data exploration** (theory, experiment & simulation)

How has science publishing changed?

nature research

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PHILOSOPHICAL

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276 NATURE [JANUARY 23, 1896

body between the source and a photographic plate or fluorescent screen.

I have observed and photographed many such shadow pictures. Thus, I have an outline of part of a door covered with lead paint; the image was produced by placing the discharge-tube on one side of the door, and the sensitive plate on the other. I have also a shadow of the bones of the hand (Fig. 1), of a wire wound upon a bobbin, of a set of weights in a box, of a

FIG. 1.—Photograph of the bones in the fingers of a living human hand. The third finger has a ring upon it.

compass card and needle completely enclosed in a metal case (Fig. 2), of a piece of metal where the X-rays show the want of homogeneity, and of other things.

For the rectilinear propagation of the rays, I have a pin-hole photograph of the discharge apparatus covered with black paper. It is faint but unmistakable.

(15) I have sought for interference effects of the X-rays,

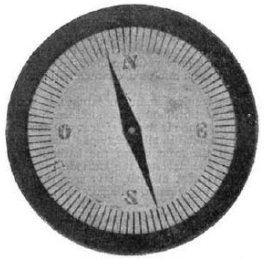

FIG. 2.—Photograph of a compass card and needle completely enclosed in a metal case.

but possibly, in consequence of their small intensity, without result.

(16) Researches to investigate whether electrostatic forces act on the X-rays are begun but not yet concluded.

(17) If one asks, what then are these X-rays; since they are not kathode rays, one might suppose, from their power of exciting fluorescence and chemical action, them to be due to ultra-violet light. In opposition to this view a weighty set of considerations presents itself. If X-rays be indeed ultra-violet light, then that light must possess the following properties.

(a) It is not refracted in passing from air into water, carbon bisulphide, aluminium, rock-salt, glass or zinc.

(b) It is incapable of regular reflection at the surfaces of the above bodies.

(c) It cannot be polarised by any ordinary polarising media.

(d) The absorption by various bodies must depend chiefly on their density.

That is to say, these ultra-violet rays must behave quite differently from the visible, infra-red, and hitherto known ultra-violet rays.

These things appear so unlikely that I have sought for another hypothesis.

A kind of relationship between the new rays and light rays appears to exist; at least the formation of shadows, fluorescence, and the production of chemical action point in this direction. Now it has been known for a long time, that besides the transverse vibrations which account for the phenomena of light, it is possible that longitudinal vibrations should exist in the ether, and, according to the view of some physicists, must exist. It is granted that their existence has not yet been made clear, and their properties are not experimentally demonstrated. Should not the new rays be ascribed to longitudinal waves in the ether?

I must confess that I have in the course of this research made myself more and more familiar with this thought, and venture to put the opinion forward, while I am quite conscious that the hypothesis advanced still requires a more solid foundation.

PROFESSOR RÖNTGEN'S DISCOVERY.

THE newspaper reports of Prof. Röntgen's experiments have, during the past few days, excited considerable interest. The discovery does not appear, however, to be entirely novel, as it was noted by Hertz that metallic films are transparent to the kathode rays from a Crookes or Hittorf tube, and in Lenard's researches, published about two years ago, it is distinctly pointed out that such rays will produce photographic impressions. Indeed, Lenard, employing a tube with an aluminium window, through which the kathode rays passed out with comparative ease, obtained photographic shadow images almost identical with those of Röntgen, through pieces of cardboard and aluminium interposed between the window and the photographic plate.

Prof. Röntgen has, however, shown that this aluminium window is unnecessary, as some portion of the kathode radiations that are photographically active will pass through the glass walls of the tube. Further, he has extended the results obtained by Lenard in a manner that has impressed the popular imagination, while, perhaps most important of all, he has discovered the exceedingly curious fact that bone is so much less transparent to these radiations than flesh and muscle, that if a living human hand be interposed between a Crookes tube and a photographic plate, a shadow photograph can be obtained which shows all the outlines and joints of the bones most distinctly.

Working upon the lines indicated in the telegrams from Vienna, recently published in the daily papers, I have, with the assistance of Mr. J. C. M. Stanton, repeated many of Prof. Röntgen's experiments with entire success. According to one of our first experiments, an ordinary gelatinous bromide dry photographic plate was placed in an ordinary camera back. The wooden shutter of the back was kept closed, and upon it were placed miscellaneous articles such as coins, pieces of wood, carbon, ebonite, vulcanised fibre, aluminium, &c., all being quite opaque to ordinary light. Above was supported a

Wilhelm Roentgen 1896

VIII. *A Dynamical Theory of the Electromagnetic Field.* By J. CLERK MAXWELL, *F.R.S.*

Received October 27,—Read December 8, 1864.

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† "Explicare tentatur
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MDCCCLXV.

Ja

equipment, and to Dr. G. E. R. Deacon and the captain and officers of R.R.S. *Discovery II* for their part in making the observations.

[1] Young, F. B., Gerrard, H., and Jevons, W., *Phil. Mag.*, **40**, 149 (1920).

[2] Longuet-Higgins, M. S., *Mon. Not. Roy. Astro. Soc., Geophys. Supp.*, **5**, 285 (1949).

[3] Von Arx, W. S., Woods Hole Papers in Phys. Oceanog. Meteor., **11** (3) (1950).

[4] Ekman, V. W., *Arkiv. Mat. Astron. Fysik.* (Stockholm), **2** (11) (1905).

MOLECULAR STRUCTURE OF NUCLEIC ACIDS

A Structure for Deoxyribose Nucleic Acid

WE wish to suggest a structure for the salt of deoxyribose nucleic acid (D.N.A.). This structure has novel features which are of considerable biological interest.

A structure for nucleic acid has already been proposed by Pauling and Corey[1]. They kindly made their manuscript available to us in advance of publication. Their model consists of three intertwined chains, with the phosphates near the fibre axis, and the bases on the outside. In our opinion, this structure is unsatisfactory for two reasons: (1) We believe that the material which gives the X-ray diagrams is the salt, not the free acid. Without the acidic hydrogen atoms it is not clear what forces would hold the structure together, especially as the negatively charged phosphates near the axis will repel each other. (2) Some of the van der Waals distances appear to be too small.

Another three-chain structure has also been suggested by Fraser (in the press). In his model the phosphates are on the outside and the bases on the inside, linked together by hydrogen bonds. This structure as described is rather ill-defined, and for this reason we shall not comment on it.

This figure is purely diagrammatic. The two ribbons symbolize the two phosphate—sugar chains, and the horizontal rods the pairs of bases holding the chains together. The vertical line marks the fibre axis

We wish to put forward a radically different structure for the salt of deoxyribose nucleic acid. This structure has two helical chains each coiled round the same axis (see diagram). We have made the usual chemical assumptions, namely, that each chain consists of phosphate diester groups joining β-D-deoxyribofuranose residues with 3′,5′ linkages. The two chains (but not their bases) are related by a dyad perpendicular to the fibre axis. Both chains follow right-handed helices, but owing to the dyad the sequences of the atoms in the two chains run in opposite directions. Each chain loosely resembles Furberg's[2] model No. 1; that is, the bases are on the inside of the helix and the phosphates on the outside. The configuration of the sugar and the atoms near it is close to Furberg's 'standard configuration', the sugar being roughly perpendicular to the attached base. There is a residue on each chain every 3·4 A. in the *z*-direction. We have assumed an angle of 36° between adjacent residues in the same chain, so that the structure repeats after 10 residues on each chain, that is, after 34 A. The distance of a phosphorus atom from the fibre axis is 10 A. As the phosphates are on the outside, cations have easy access to them.

The structure is an open one, and its water content is rather high. At lower water contents we would expect the bases to tilt so that the structure could become more compact.

The novel feature of the structure is the manner in which the two chains are held together by the purine and pyrimidine bases. The planes of the bases are perpendicular to the fibre axis. They are joined together in pairs, a single base from one chain being hydrogen-bonded to a single base from the other chain, so that the two lie side by side with identical *z*-co-ordinates. One of the pair must be a purine and the other a pyrimidine for bonding to occur. The hydrogen bonds are made as follows: purine position 1 to pyrimidine position 1; purine position 6 to pyrimidine position 6.

If it is assumed that the bases only occur in the structure in the most plausible tautomeric forms (that is, with the keto rather than the enol configurations) it is found that only specific pairs of bases can bond together. These pairs are: adenine (purine) with thymine (pyrimidine), and guanine (purine) with cytosine (pyrimidine).

In other words, if an adenine forms one member of a pair, on either chain, then on these assumptions the other member must be thymine; similarly for guanine and cytosine. The sequence of bases on a single chain does not appear to be restricted in any way. However, if only specific pairs of bases can be formed, it follows that if the sequence of bases on one chain is given, then the sequence on the other chain is automatically determined.

It has been found experimentally[3,4] that the ratio of the amounts of adenine to thymine, and the ratio of guanine to cytosine, are always very close to unity for deoxyribose nucleic acid.

It is probably impossible to build this structure with a ribose sugar in place of the deoxyribose, as the extra oxygen atom would make too close a van der Waals contact.

The previously published X-ray data[5,6] on deoxyribose nucleic acid are insufficient for a rigorous test of our structure. So far as we can tell, it is roughly compatible with the experimental data, but it must be regarded as unproved until it has been checked against more exact results. Some of these are given in the following communications. We were not aware of the details of the results presented there when we devised our structure, which rests mainly though not entirely on published experimental data and stereochemical arguments.

It has not escaped our notice that the specific pairing we have postulated immediately suggests a possible copying mechanism for the genetic material.

Full details of the structure, including the conditions assumed in building it, together with a set of co-ordinates for the atoms, will be published elsewhere.

We are much indebted to Dr. Jerry Donohue for constant advice and criticism, especially on interatomic distances. We have also been stimulated by a knowledge of the general nature of the unpublished experimental results and ideas of Dr. M. H. F. Wilkins, Dr. R. E. Franklin and their co-workers at

Watson & Crick 1953

Changing paradigm

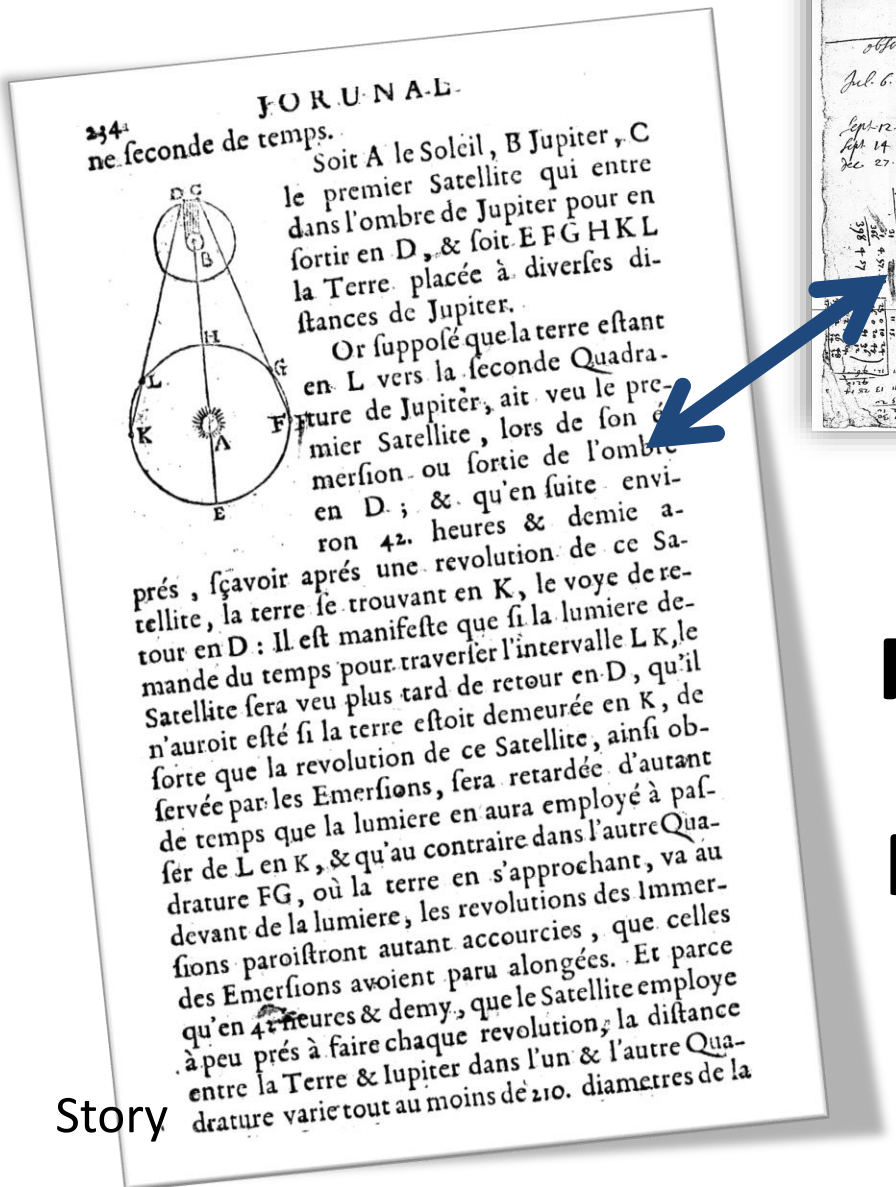
The old type of narrative:

data to support a hypothesis

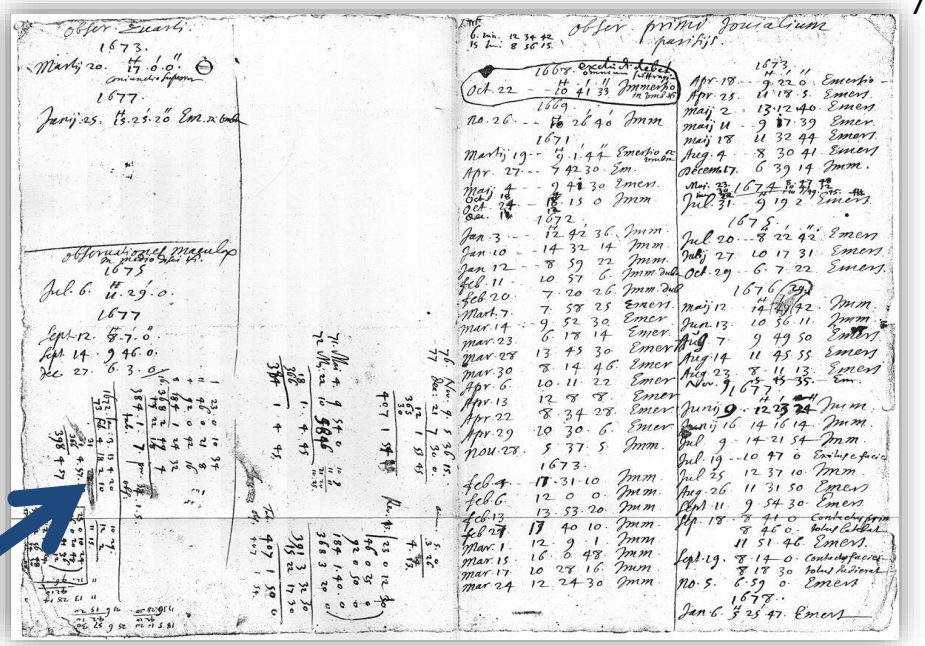
Data-intensive science:

- Large amounts of data
- Should be made accessible to others
- Exploratory use

data interesting in itself


234 JORUNAL
ne seconde de temps.
Soit A le Soleil, B Jupiter, C le premier Satellite qui entre dans l'ombre de Jupiter pour en sortir en D, & soit EFGHKL la Terre placée à diverses distances de Jupiter.
Or supposé que la terre estant en L vers la seconde Quadrature de Jupiter, ait veu le premier Satellite, lors de son émersion ou sortie de l'ombre en D; & qu'en suite environ 42. heures & demie aprés, sçavoir aprés une revolution de ce Satellite, la terre se trouvant en K, le voye de retour en D: Il est manifeste que si la lumiere demande du temps pour traverser l'intervalle LK, le Satellite sera veu plus tard de retour en D, qu'il n'auroit esté si la terre estoit demeurée en K, de sorte que la revolution de ce Satellite, ainsi observée par les Emersions, sera retardée d'autant de temps que la lumiere en aura employé à passer de L en K, & qu'au contraire dans l'autre Quadrature FG, où la terre en s'approchant, va au devant de la lumiere, les revolutions des Immersions paroistront autant accourcies, que celles des Emersions avoient paru alongées. Et parce qu'en 42 heures & demy, que le Satellite employe à peu prés à faire chaque revolution, la distance entre la Terre & Iupiter dans l'un & l'autre Quadrature varie tout au moins de 210. diametres de la

Story



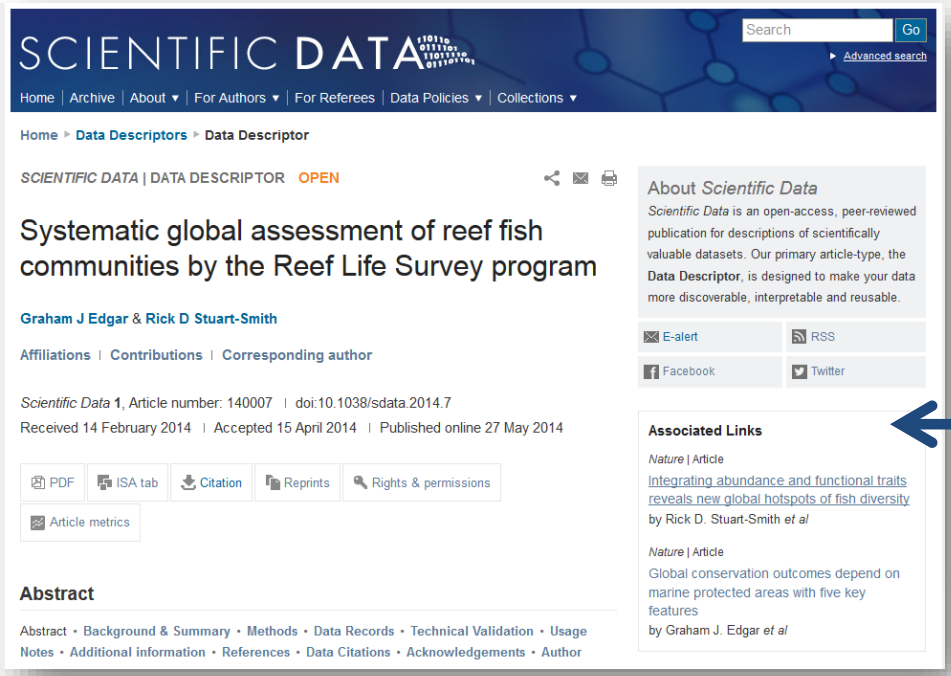
Data

Filter and publish?
or
Publish and filter?

nature research

A possible answer: data journals

- *Scientific Data* (NPG)
- *Data in Brief*, *Genomics Data* (Elsevier)
- *Geoscience Data Journal* (Wiley)



nature research

The concept of Data journals

- Data must be well described before others can use it and benefit from it
- Scientists who share data in a reusable manner deserve credit through citable publications
- Data quality matters

nature research

How does it work?

- Include methods and technical analyses supporting the quality of the data
- Publish alongside a journal article
- Describe standalone datasets that don't fit in other publications
- Release data used in previous research articles

www.nature.com/scie

SCIENTIFIC DATA

OPEN

Data Descriptor: High-through DFT calculations of formation energy, stability and oxygen vacancy formation energy of A perovskites

Received: 26 May 2017
Accepted: 22 August 2017
Published: 17 October 2017

Antoine A. Emery[1] & Chris Wolverton[1]

ABO_3 perovskites are oxide materials that are used for a variety of applications such as solid o piezo-, ferro-electricity and water splitting. Due to their remarkable stability with respect to substitution, new compounds for such applications potentially await discovery. In this work, exhaustive dataset of formation energies of 5,329 cubic and distorted perovskites that were using first-principles density functional theory. In addition to formation energies, several ad properties such as oxidation states, band gap, oxygen vacancy formation energy, and therm stability with respect to all phases in the Open Quantum Materials Database are also made available. This large dataset for this ubiquitous crystal structure type contains 395 perovskit predicted to be thermodynamically stable, of which many have not yet been experimentally therefore represent theoretical predictions. The dataset thus opens avenues for future use, materials discovery in many research-active areas.

Design Type(s)	database creation objective
Measurement Type(s)	physicochemical characterization
Technology Type(s)	computational modeling technique
Factor Type(s)	compound by chemical composition
Sample Characteristic(s)	

Data in Brief 14 (2017) 453–457

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

Dataset on electro-optically tunable smart-supercapacitors based on oxygen-excess nanograin tungsten oxide thin film

Akbar I. Inamdar [a,*], Jongmin Kim [a], Yongcheol Jo [a], Hyeonseok Woo [a], Sangeun Cho [a], Sambhaji M. Pawar [a], Seongwoo Lee [a], Jayavant L. Gunjakar [a], Yuljae Cho [b], Bo Hou [b], Seung Nam Cha [b], Jungwon Kwak [c], Youngsin Park [d], Hyungsang Kim [a,*], Hyunsik Im [a,*]

[a] Division of Physics and Semiconductor Science, Dongguk University, Seoul 04620, South Korea
[b] Department of Engineering Science, University of Oxford, Parks Road, OX1 3PJ, UK
[c] Medical Physics Department, Asan Medical Center, Seoul, South Korea
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Keywords:
Multi-functional electrode
Oxygen-excess tungsten oxide
Nanograin
Electrochromism
Supercapacitor

ABSTRACT

The dataset presented here is related to the research article entitled "Highly Efficient Electro-optically Tunable Smart-supercapacitors Using an Oxygen-excess Nanograin Tungsten Oxide Thin Film" (Akbar et al., 2017) [9] where we have presented a nanograin WO_3 film as a bifunctional electrode for smart supercapacitor devices. In this article we provide additional information concerning nanograin tungsten oxide thin films such as atomic force microscopy, Raman spectroscopy, and X-ray diffraction spectroscopy. Moreover, their electrochemical properties such as cyclic voltammetry, electrochemical supercapacitor properties, and electrochromic properties including coloration efficiency, optical modulation and electrochemical impedance spectroscopy are presented.

DOI of original article: http://dx.doi.org/10.1016/j.solmat.2017.03.006
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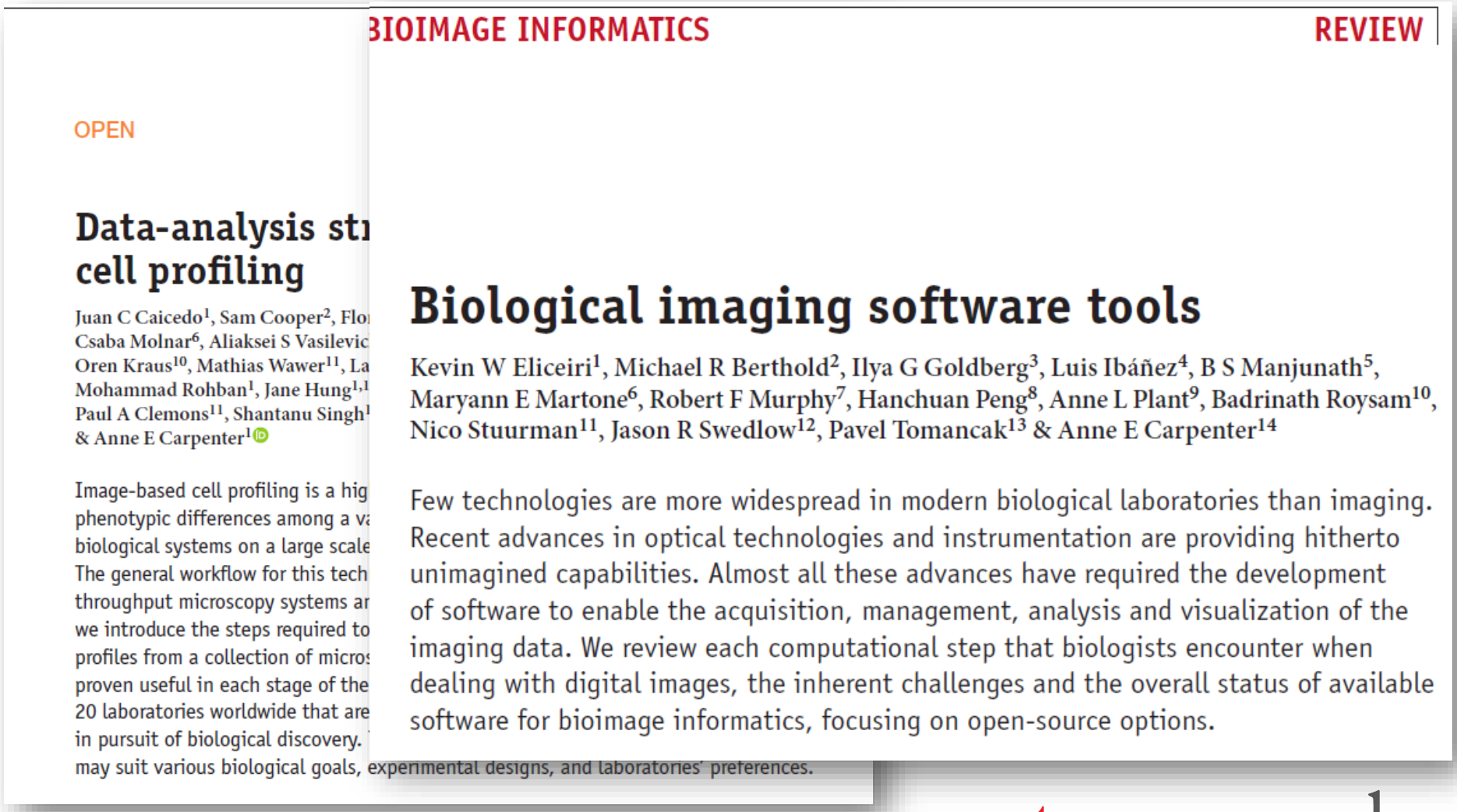
http://dx.doi.org/10.1016/j.dib.2017.07.051
2352-3409/

How about data & software reviews?



OPEN

Data-analysis str
cell profiling

Juan C Caicedo[1], Sam Cooper[2], Flo
Csaba Molnar[6], Aliaksei S Vasilevic
Oren Kraus[10], Mathias Wawer[11], La
Mohammad Rohban[1], Jane Hung[1,1
Paul A Clemons[11], Shantanu Singh[1
& Anne E Carpenter[1]

Image-based cell profiling is a hig
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The general workflow for this tech
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proven useful in each stage of the
20 laboratories worldwide that are
in pursuit of biological discovery.
may suit various biological goals, experimental designs, and laboratories' preferences.

BIOIMAGE INFORMATICS REVIEW

Biological imaging software tools

Kevin W Eliceiri[1], Michael R Berthold[2], Ilya G Goldberg[3], Luis Ibáñez[4], B S Manjunath[5], Maryann E Martone[6], Robert F Murphy[7], Hanchuan Peng[8], Anne L Plant[9], Badrinath Roysam[10], Nico Stuurman[11], Jason R Swedlow[12], Pavel Tomancak[13] & Anne E Carpenter[14]

Few technologies are more widespread in modern biological laboratories than imaging. Recent advances in optical technologies and instrumentation are providing hitherto unimagined capabilities. Almost all these advances have required the development of software to enable the acquisition, management, analysis and visualization of the imaging data. We review each computational step that biologists encounter when dealing with digital images, the inherent challenges and the overall status of available software for bioimage informatics, focusing on open-source options.

nature research

Coming up in *Nature Reviews Physics* in 2019

The future

- Publishing data & software will become more widespread
- Scientists and funders will come to appreciate these new articles on the same footing as primary research
- **Challenges**: educating scientists to write and peer-review these new articles and establish guidelines for good scientific practice