Blockchain Technology and its Use Along the Scientific Research Workflow

A IUPAC White Paper Coming Soon

by Bonnie Lawlor, Stuart Chalk, Jeremy Frey, Kazuhiro Hayashi, David Kochalko, Richard Shute, and Mirek Sopek

At the Council meeting held during the 2019 World Chemistry Congress in Paris, a representative from one of IUPAC's National Adhering Organizations raised the question "What is Blockchain Technology?" They went on to say that both "Blockchain" and "Artificial Intelligence" were prominent buzzwords and asked if IUPAC could provide information on how these technologies were impacting science in general and chemistry in particular. Coincidentally, at that same Congress, the technology had been the subject of a presentation by Richard Shute [1], one of the authors of this paper, and the technology had already captured the interest of Bonnie Lawlor, another of the authors of this paper, to the extent that she published an article in *Chemistry International (CI)* on the topic the following year [2]. As a result of the question raised at the Council meeting, Javier García-Martínez, IUPAC President 2022-2023, suggested that a white paper on Blockchain be developed (Note: Artificial Intelligence was made the focus of the global, virtual 2021 World Chemistry Leadership Meeting (WCLM) and a brief article on that special event was published in the July 2022 issue of *CI* [3]).

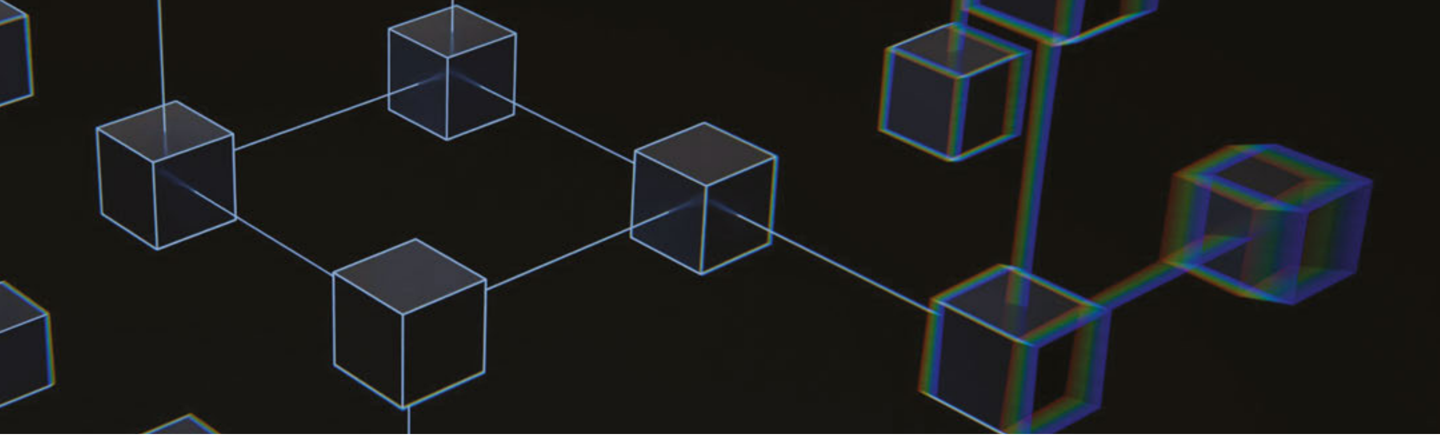
While not a technologist herself, Lawlor agreed to organize a team of experts to develop a white paper on the technology, and in 2020 the group began interviewing experts around the world and researching how the technology is being applied along the scientific research workflow. Over the next few pages, we want to provide a high-level overview of what you can expect when the paper is published in *Pure and Applied Chemistry* in the coming months. The paper will drill down in much more detail, plus provide a wealth of reading material for those interested in learning more.

What is Blockchain?

In its current iteration, what is commonly referred to as "the blockchain" is a platform that can be used to support many diverse applications. While this new technology gained popularity because of its use by a community of those interested in cryptocurrencies, specifically Bitcoin [4], the technology is simply the engine "under the hood" of Bitcoin—an engine that can be used for other purposes as well. Indeed, "Blockchain is to Bitcoin, what the Internet is to email. A big electronic system, on top of which you can build applications. Currency is just one." [5] In fact, blockchain technology actually predates Bitcoin by almost twenty years. It was co-invented in 1991 by Stuart Haber and W. Scott Stornetta who both worked at Bell Communications Research (Bellcore) and who were attempting to ensure the integrity of digital records via time stamping. They believed that the ability to certify when a document was created or last modified would be essential to the resolution of conflicts over such things as intellectual property rights.

Their initial efforts involved working on a cryptographically-secured chain of blocks such that no one could tamper with the timestamps of documents. Within a year they upgraded the efficiency of their system by incorporating Merkle trees [6], enabling the collection of more documents on a single block [7]. The Merkle trees created a series of data records, each connected to the one before it. The newest record in the chain would contain the history of the entire chain, making it more efficient by allowing several documents to be collected into one block [8]. Hence the name "Blockchain." (Note: the technology is also referred to as distributed ledger technology (DLT) due to its similarity to the double-entry book-keeping [9] method that dates to the fourteenth century).

The blocks record and confirm the time and sequence of transactions and each block contains a digital fingerprint or unique identifier (a "hash"), time-stamped batches of recent valid transactions, and the hash of the previous block. The hash of the previous block links the blocks together and prevents any block from being altered or a block being inserted between two existing blocks. Each subsequent block strengthens the verification of the previous block and hence the



entire blockchain. The method renders the blockchain tamper-evident, lending to the key attribute of immutability [10]. Time stamping even today remains one of the more common applications of the technology and the technology is becoming widely-used by researchers to protect their work and provide proof-of-concept and intellectual property ownership (data provenance).

Haber and Stornetta left Bellcore in 1994 to co-found a spin-off company, Surety, which provided time-stamping services based upon their algorithms and it was the first company to provide commercial blockchain-based services [11]. Things remained quiet on the blockchain front until 2008 when Satoshi Nakamoto released a white paper entitled, "Bitcoin: a peer-to-peer electronic cash system," which proposed a system of electronic transactions that did not require a reliance upon trust—the middleman (*e.g.* a bank) was removed [12]. Haber and Stornetta's seminal paper, "How to Time-Stamp a Digital Document," [13] is referenced in the Bitcoin white paper. To this day no one knows anything about Nakamoto—whether it is a single person or a research group, and he/she/they left the Bitcoin community in about 2010, leaving blockchain technology development in the hands of those passionate about the technology—computer scientists, cryptographers, and mathematicians around the world [14].

The Importance of Blockchain Technology to Science

Over the years since Nakamoto built upon Haber and Stornetta's work there have been a series of enhancements to blockchain technology, primarily driven by the realization that the technology did *not* need to be tethered to Bitcoin—it could be used for all sorts of cooperative efforts between organizations—including scientific research.

According to a report from the National Institute of Standards and Technology (NIST), "Blockchains are immutable digital ledger systems implemented in a distributed fashion (*i.e.,* without a central repository) and usually without a central authority. At its most basic level, they enable a community of users to record transactions in a ledger public to that community such that no transaction can be changed (fraudulently) once published." [15]

In addition, a recent report from the European Chemical Industry Council, "Artificial Intelligence and Blockchain: Insights and Actions for the Chemical Industry," [16] states that blockchain technology holds the potential for disruption across the chemical enterprise—both along a company's internal scientific research and development workflow and externally along a company's manufacturing supply chain to end-user consumption. The technology is important for many reasons, but the primary reason is that it provides incontrovertible proof-of-creation of an idea, research data, *etc.* Once linked to a blockchain and time-stamped, the data can be changed, but such changes are captured and time-stamped, making fraudulent tampering visible. This makes digital goods immutable, transparent, externally-provable, decentralized, and distributed. Consequently, blockchain technology could do much to mitigate the inability to duplicate research results.

According to Sönke Bartling (Mannheim University), all parts of the research cycle could take place within a blockchain system [17]. Attribution, data, data post-processing, publication, research evaluation, incentivization, and research fund distribution could thereby become comprehensible, open (at will), and provable to the external world. It would make more of the research cycle open to audited scientific correction and eliminate duplicative research. Bartling believes that it can potentially open the way to true collaborative, real-time research, thus expediting the advancement of science. A secondary reason for the importance of blockchain is that it allows the attachment of formal terms of agreement with digital goods, *e.g.,* licenses, usage limitations, smart contracts, *etc.* In addition, it also holds the potential for creating totally new business models, for reducing administrative and labor costs, and for providing rewards for work performed, such as for peer review in scholarly communication.

While use of blockchain technology beyond its original association with bitcoin is still in its early stages, there has been increased experimentation and adoption of the technology during the last six years. Those closely monitoring its adoption and the emergence of new use cases predicted that the rate of adoption would increase once Ethereum 2.0 (one of the major blockchain technologies) was released. As expected, the new release is mitigating several obstacles to blockchain adoption— speed, cost, and scalability [18]. Indeed, Universities are beginning to focus on the technology to foster innovative research. Two examples in the USA are Stanford University's Stanford Center for Blockchain Research and the Walton College Blockchain Center for Excellence at the University of Arkansas. A European example is the Open University in the UK who is a member of the Bloxberg Consortium and who uses their blockchain for several blockchain-related research projects.

To quote the aforementioned report from the European Chemical Industry Council, "Blockchain is still an emerging technology and its use in the chemical industry is limited. But early proof-of-concept applications in other industries have already illustrated its benefits and are now moving to market adoption… blockchain is moving ahead quickly, but adoption will take time and effort. Chemical companies should start now to understand the benefits and develop a plan to incorporate it into their organization (where appropriate)."

Current Applications

As noted earlier, the objective of the white paper is to demonstrate how blockchain technology is being used along the scientific research workflow which has been defined as having the following five steps:

- Step #1: Develop Hypothesis/Define an idea;
- Step #2: Seek Funding (if needed);
- Step #3: Perform the Experiment/make observations;
- Step #4: Perform analysis/make insights;
- Step #5: Publish/share results.

The authors of this paper have held about a dozen in-depth interviews with major global players across diverse disciplines who are successfully using blockchain technology for a variety of purposes in the scientific workflow and the white paper will provide details on these uses. A sampling of the applications includes the following use cases:

- Time-stamping of data, ideas, etc. to provide proof-of-concept and intellectual property ownership (data provenance)
- Data sharing within closed networks/communities
- Near real-time research tracking (e.g., Covid-19 tracking is done via blockchain by the U.S. Department of Health and Human Services; the same can be applied to any research having global priorities)
- Authentication of data at the source for auditing, compliance, and regulatory purposes
- Equipment management (maintenance records, training, usage history, ownership history, etc.)—can even ensure compliance with the Good Manufacturing Practices required by regulatory agencies
- Supply-chain tracking for both tangible/physical and digital/data assets
- Decentralized publishing/peer review
- Research Funding/tracking
- Crowd-sourcing/collaborative research (both public and within companies) where blockchain helps to confirm who owns what because it can demonstrate who did what
- Degree and qualification certification
- Identity certification of people and objects
- Research data re-use (including sales of such data)
- Retrieval of chemicals/pharmaceuticals at the end of their life cycles or during their life cycle for re-purposing
- Digital asset ownership using non-fungible tokens (NFTs).

Some of this activity is commercial (for-profit) and other applications are in the academic/non-profit market sector as well as in government sectors. A few examples of organizations using the technology are as follows:

ARTiFACTS: Established in 2018, this is a for-profit organization that uses the Bloxberg Consortium blockchain to ensure provenance of research along the scientific workflow, from time stamping of ideas/research, data sharing, through to publishing (see: https://artifacts.ai). More recently, ARTiFACTS has partnered with Marya Lieberman and the Distributed Pharmaceutical Analysis Lab (DPAL) at the University of Notre Dame to develop a prototype solution for tracking pharmaceutical chain-of-custody information in real-time using distributed ledger technology. Working with ARTiFACTS, DPAL records all physical handling and research metadata starting from the point-of-purchase of prescription drugs and sustained throughout the testing, analysis, and reporting requirements.

Bloxberg Consortium (out of the Max Planck Digital Library (MPDL)): Formally established in February 2019, MPDL has created a non-profit global network for the use of blockchain technology. Members of this network operate the nodes of a blockchain ledger for the development and deployment of diverse services and use cases in support of research. The number of members has grown from the original eleven to more than fifty and will likely increase as the pandemic winds down and in-person meeting return. This consortium is being perceived as the blockchain for science and is used across diverse scientific disciplines, including chemistry (see: https://bloxberg.org). It should be noted that at the fourth Bloxberg Summit meeting held 4-5 May 2022 more than twenty-five research organizations decided on several proposals regarding the future development of the Bloxberg network. They made a groundbreaking decision, introducing a significant and forward-looking change for the future of the network: the "Bloxberg Association for the Advancement of Blockchain in Science" which was founded under German legislation that same year [19].

Open Science Chain (OSC): Launched in 2018, this is a consortium blockchain (like Bloxberg) that is funded by the U.S National Science Foundation (Award: 1840218 [20]) and is based at the San Diego Supercomputer Center at the University of California San Diego. Its main objective is to support data sharing to enable independent verification of scientific data and to foster reuse for the advancement of science (see: https://opensciencechain.org). They provide for the time stamping of datasets along with data ownership; promote the transparency and traceability of research data by tracking and storing all changes made to the data on the blockchain; and allow for independent verification of the authenticity of scientific data using information stored in the OSC blockchain. The project has been successful and, in the summer of 2021, received an additional half million dollars from the NSF for expansion [21]. The service is free to members of the academic and research communities. For more information about the OSC mission see its seminal paper [22].

U.S. Health and Human Services (HHS): Uses blockchain technology to reduce the time required to find the best deal for purchases of equipment, clinical tools, *etc.* This regularly could take four to five months and their new service, Accelerate, allows people to find what they needed in real time. After the success of Accelerate, HHS almost immediately initiated a pilot, the Grant-recipient Digital Dossier (GDD), to manage their grant program more efficiently. As of July 2021, GDD has reduced the time required to complete grant assessment tasks from four-plus-hours to a fifteen-minute process [23].

The white paper will include other examples, including those in areas such as education and identity management.

Other Areas Covered

The white paper also includes a section on legal and regulatory issues related to blockchain technology. What this section attempts to offer is some background on legislation and regulation as it currently applies to blockchain technology for organizations who actually want to "use" the technology—basically what you need to learn more about before venturing in. There is also a section on the current developments to improve the technology as well as what readers can expect in the not-too-distant future along with an extensive reading list.

A clear conclusion is that the use of the technology is not for everyone, and is not the solution to every problem. The white paper also provides examples of where the technology has failed, and why. The authors concur with the following statement from the NIST report mentioned earlier: "The use of blockchains is still in its early stages, but it is built on widely-understood and sound cryptographic principles. Moving forward, it is likely that blockchains will be another tool that can be used to solve newer sets of problems…To avoid missed opportunities, organizations should start investigating whether or not a blockchain can help them." [24] What we learned from our interviews is that usage of the technology is growing in general and is accelerating in the life and health sciences. We found that Sönke Bartling is right - all parts of the research cycle *can* take place within a blockchain system. We expect new developments to emerge, and we plan to update the white paper at regular intervals as the technology is enhanced and new use cases and new players emerge. In fact, a recent report from the Davos 2023 World Economic Forum states that "blockchain technology offers more promises than problems and that as a technology it will continue to grow exponentially, and its use cases expand. The real-world applications of blockchain, many already in use by organizations focused on international development, offer greater utility and cost savings." [25]

In closing we believe that the future of blockchain technology looks bright. While the scope of its impact is hard to predict as it is in the early stages of broad adoption, according to Gartner, Inc., a market research company that follows the rise (and fall) of technologies, "The evolution of blockchain cannot be ignored…The impact of the technology will be significant." [26] (*Note:* Blockchain Technology was selected as one of the Top Ten Emerging Technologies in Chemistry in 2021. An article on those technologies appears in the October 2021 issue of *Chemistry International.* [27])

Notes and References

. (all accessed 1 May 2024)

1. Shute, R. E., "Blockchain and Distributed Ledger Technology: Enhancing Trust in Science," 2019; see the slides at: https://www.slideshare.net/RichardShute1/blockchain-and-distributed-ledger-technology-enhancing-trust-in-science
2. Lawlor, B., "Blockchain Technology: Uses in Research and Communication" *Chem. Int.* 2020, 42(3), 8-11; https://doi.org/10.1515/ci-2020-0304
3. Frey, J., Lawlor, B., McEwen, L., Ober, C., Williams, A., "A Global Conversation on the Use of Artificial Intelligence in Chemistry," *Chem. Int.2022*, 44(3), 8-11; https://doi.org/10.1515/ci-2022-0303
4. See "What is Bitcoin": https://www.bitcoin.com/get-started/what-is-bitcoin/
5. Davies, S., "How Bitcoin and its Blockchain Works," *Financial Times*, video, February 3, 2015, see: https://www.ft.com/video/2be94381-66dc-3320-a292-6a1cde0a3d5f
6. Merkle tree, Wikipedia, https://en.wikipedia.org/wiki/merkle_tree
7. Iredale, G., "History of Blockchain Technology: A Detailed Guide," 3 Nov 2020, see: https://101blockchains.com/history-of-blockchain-timeline
8. Lytovchenko, A., The History of Blockchain: From Establishment to Broad Adoption, eleks, 8 May 2020, updated 5 March 2021, see https://eleks.com/blog/the-history-of-blockchain/
9. Double Entry Bookkeeping, Wikipedia, https://en.wikipedia.org/wiki/double_entry_bookkeeping
10. Gupta, M., Blockchain for Dummies," IBM, 3rd edition released 2020, p. 13, see: https://www.ibm.com/topics/what-is-blockchain
11. See: https://www.worldcryptoindex.com/creators/w-scott-stornetta/
12. Nakamoto, S., "Bitcoin: a peer-to-peer electronic cash system," 2009, see: https://www.bitcoin.com/bitcoin.pdf
13. Haber, S., Stornetta, W. S., "How to Time-Stamp a Digital Document," *The Journal of Cryptology 1991*, 3(2), 99-111, 1991; https://doi.org/10.1007/BF00196791
14. Redman, J., "Bitcoin's Creator Satoshi Nakamoto is Now a Member of the Top 20 World's Richest People," Bitcoin.com, 12 April 2021, see: https://news.bitcoin.com/bitcoins-creator-satoshi-nakamoto-now-a-member-top-20-worlds-richest-people/
15. Yaga, D., Mell., P., Roby, N., Scarfone, K., *NISTIR 8202 Blockchain Technology Overview,* National Institute of Standards and Technology, U. S. Department of Commerce, January 2018, https://arxiv.org/abs/1906.11078
16. See: AI and Blockchain in the Chemical Industry, Accenture, June 2019; https://www.accenture.com/us-en/insights/chemicals/ai-blockchain-chemical-industry
17. Bartling, S., Fecher, B., "Blockchain for science and knowledge creation," 2016, https://doi.org/10.5281/zenodo.60223
18. See: https://www.forbes.com/advisor/in/investing/cryptocurrency/what-is-ethereum-2-merge/
19. See press release at: https://www.mpdl.mpg.de/ueber/presse/812-fourth-bloxberg-summit-2022.html
20. See: https://www.nsf.gov/awardsearch/showAward?AWD_ID=1840218
21. Bruch, K. M., SDSC's Open Science Chain Awarded $500,000 NSF Grant, 3 Aug 2021; see: https://www.sdsc.edu/News%20Items/PR20210803_opensciencechain.html
22. Sivagnanam, S., Nandigam, V., Lin, K., "Introducing the Open Science Chain: Protecting Integrity and Provenance of Research Data," Proceedings of the Practice and Experience in Advanced Research Computing on Rise of the Machines (learning), Association for Computing Machinery (ACM), p. 18, July 2019.
23. Harris, M., "How Blockchain is Transforming Grants Management," Government CIO Media and Research, 27 July 2021; see: https://governmentciomedia.com/how-blockchain-transforming-federal-grants-management
24. Yaga, D., Mell., P., Roby, N., Scarfone, K., *NISTIR 8202 Blockchain Technology Overview,* National Institute of Standards and Technology, U. S. Department of Commerce, Jan 2018.
25. A. Nath, In Davos, Blockchain Yields More Promises Than Problems, https://www.coindesk.com/consensus-magazine/2023/01/18/in-davos-blockchain-yields-more-promises-than-problems/
26. Furlonger, D., Uzureau, C., *The Real Business of Blockchain: How Leaders can Create Value in a New Digital Age*, Gartner, Inc., Harvard Review Press, Boston, Massachusetts, USA, 2019, ISBN: 9781633698048.
27. Gomollón-Bel, Fernando. "IUPAC Top Ten Emerging Technologies in Chemistry 2021: Breakthroughs for a circular, climate-neutral future" *Chem. Int. 2021*, 43(4), 13-20; https://doi.org/10.1515/ci-2021-0404

The White Paper in *Pure and Applied Chemistry* is scheduled to be released ahead of print in the coming weeks; check https://www.degruyter.com/pac

See also https://iupac.org/project/2023-009-1-024/ for details.

Bonnie Lawlor, Chair, CPCDS Subcommittee on Publications;
Stuart Chalk, Professor of Chemistry, University of North Florida;
ORCID 0000-0002-0703-7776
Jeremy Frey, Professor of Physical Chemistry, University of Southampton;
ORCID 0000-0003-0842-4302
Kazuhiro Hayashi, Director of Research Unit for Data Application, Japanese National Institute of Science and Technology Policy;
ORCID 0000-0003-1996-4259
David Kochalko, Co-founder, ARTiFACTS;
ORCID 0000-0002-3331-2751
Richard Shute, Research Consultant, Curlew Research;
ORCID 0000-0001-5626-4281
Mirek Sopek, Chief Technology Officer, MakoLab SA;
ORCID 0000-0003-0378-5125

IUPAC2025

KUALA LUMPUR, MALAYSIA

50th World Chemistry Congress (50WCC)
13 - 18th July 2025

53rd IUPAC General Assembly (53GA)
11 - 15th July 2025

INSTITUT KIMIA MALAYSIA

IUPAC
INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

We welcome you to enchanting Malaysia!