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Guidelines for hardware-focused articles

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In this editorial, we set expectations and requirements for hardware-focused articles to *Digital Discovery*. We discuss the four criteria that should be addressed by authors and reviewers: (1) relevance to the digitalization of chemical research (broadly defined); (2) comparative analysis of the hardware to existing alternatives; (3) replicability and modification of the design; (4) instructions for operation and safety.

The journey towards realizing autonomous labs is a challenging yet rewarding interdisciplinary endeavor. The integration, instrumentation, and often, the innovative design and construction of hardware, are crucial stepping stones in this journey. However, a palpable challenge looms in the form of a glaring absence of "mainstream" materials-science or chemistry journals that cater to researchers engrossed in autonomous research integration, instrumentation, and hardware. Too often, the description of discovery-enabling hardware is tethered to a larger scientific demonstration project. This inadvertently creates a bottleneck, hindering the flow of innovation and collaborative efforts essential for advancing this domain.

The interdisciplinary expansion of digital transformation within chemical and material science has necessitated a greater emphasis on articles dedicated to hardware advancements. *Digital Discovery* has witnessed a surge in submissions of hardware articles, alongside an influx of author and reviewer queries regarding the journal's expectations in this domain. In this editorial we address those questions and set expectations and requirements for submissions describing discovery-enabling hardware. Establishing a peer-reviewed forum for these works serves a dual purpose: it assures readers of the relevance, capability, feasibility, and usability of the hardware in a scientific setting, and it also recognizes the genuine scholarly contributions of hardware development in this emerging field of automated and autonomous research.

While there exist other peer-reviewed journals dedicated to open-source and scientific instrumentation, such as **Journal of Open Hardware**, **HardwareX** and **Review of Scientific Instruments**, we envision *Digital Discovery* as specializing in open-source scientific instrumentation that propels digitalization, automation, and autonomy specifically in the realms of chemistry, materials research, and biotechnology. To maintain a high standard of scholarly contribution and to ensure a clear focus on advancing the field of autonomous chemistry and materials research, hardware articles submitted to *Digital Discovery* must address four criteria that are central to our evaluation process, assisting both the authors and reviewers in aligning with the journal's ethos of fostering innovation, replicability, and safe practices in hardware development tailored for autonomous research.

1. Relevance and advancement

- Why is this hardware significant to chemistry, materials, and/or biotechnology research (broadly defined)?

- How does it further digitalization, automation, and/or autonomy within these realms?

Authors should begin by briefly outlining the context of their work, providing citations to relevant primary or review articles that elucidate the general problem and its significance for a broader audience. Following this, authors should articulate how their work advances digitalization, data science, automation, and/or autonomous research in their respective field.

2. Comparative analysis

- How does the hardware compare to existing alternatives?

- In what aspects is it superior or inferior to those alternatives?

Authors should compare their hardware project with other commercial or do-it-yourself (DIY) alternatives, enabling readers to gauge the relevance of the hardware for their own research endeavors. This comparison should encompass, at a minimum, an analysis of capabilities, cost, adaptability, and construction time, while also possibly delving into other pertinent metrics and sub-metrics germane to the work at hand. In many instances, the available options delineate a Pareto front, with no single device unequivocally outperforming the others across all metrics. Authors should justify the trade-offs inherent in their design, identifying the scenarios where their hardware emerges as the best, an acceptable, or a less favorable option in comparison to the alternatives. This will provide a comprehensive insight into the value proposition of their hardware project, fostering a more informed and engaged readership.

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3. Replicability and modification

- Can other individuals construct and modify the hardware?

- Is the design replicable, fostering further innovation and adaptation?

Reviewers should evaluate the clarity of the build instructions and offer suggestions for enhancing the quality and relevance of both the final product and the pathway towards its construction. While complete replication of the work by constructing the hardware may be impractical for reviewers, data and code reviewers should verify that the files are free of errors (*e.g.*, mesh errors in STL files) and contain the relevant content.

In addition to any finished products, authors should provide relevant files in an editable format. For example, authors should provide editable Computed Aided Design (CAD) files in addition to finished 3d models, program source code in addition to precompiled binaries, *etc.* We acknowledge that proprietary CAD formats may exclude certain readers from adapting the work, but in general have no explicit preference for specific design software. To enable reuse, a clear license should be provided for the materials.

For hardware, we have a strong preference for open source hardware licenses, such as the CERN Open Hardware License (**http://www.ohwr.org/projects/cernohl/wiki**). For software elements, we have a strong preference for permissive open source licenses, such as the MIT or Apache license.

Patented designs may be published, provided that terms of reuse and modification are clearly indicated.

Submissions that document independent builds of the hardware performed at different sites or by different staff members provide strong evidence of replicability. For example, the work of Keesey *et al.*,[1] where the hardware was built in different forms at three different sites, demonstrates both replicability and adaptability.

While the main manuscript may be concise, it should be accompanied by detailed supporting information, including a comprehensive bill of materials and construction guide. This supporting information should enable a typical researcher—notionally a graduate student in chemistry, materials science, or biotechnology—to construct the device. All design files and software code should be hosted in a public, persistent repository, ensuring easy access and longevity of the resources. We suggest authors adopt a standard similar to DIY publications such as **Instructables.com**, which ensures a level of clarity, detail, and accessibility in the presentation of the construction guide and supporting materials. The IKEA-style instructions provided as the ESI of Chitre *et al.* is a possible example of how this could be presented.[2]

4. Operation and safety

- How will users know they have built the hardware correctly?

- Are there clear guidelines and precautions outlined for safe operation and handling?

Authors must provide a minimal "hello world" style example experiment to illustrate the device's capabilities, serving as an initial test for readers who have replicated the hardware. This may require defining a specific laboratory protocol in narrative form and/or furnishing computer code or data input files essential for conducting the demonstration. Additionally, a discussion addressing the safety and hazards associated with the construction and operation of the hardware device is expected, ensuring that users are well-informed of any risks and precautionary measures.

Next steps

We are opening a call for submissions that follow the outlined criteria focusing on relevance, replicability, comparative analysis, and safety in their hardware-centric submissions to *Digital Discovery*. We will highlight these explorations in hardware development through a themed collection on "Hardware Advancing the Digitalization of Chemistry, Materials Science, and Biotechnology."

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References

1 R. Keesey, *et al.*, *Digital Discovery*, 2023, **2**, 422–440.
2 A. Chitre, *et al.*, *Chem. Methods*, 2023, **4**, e202300043.