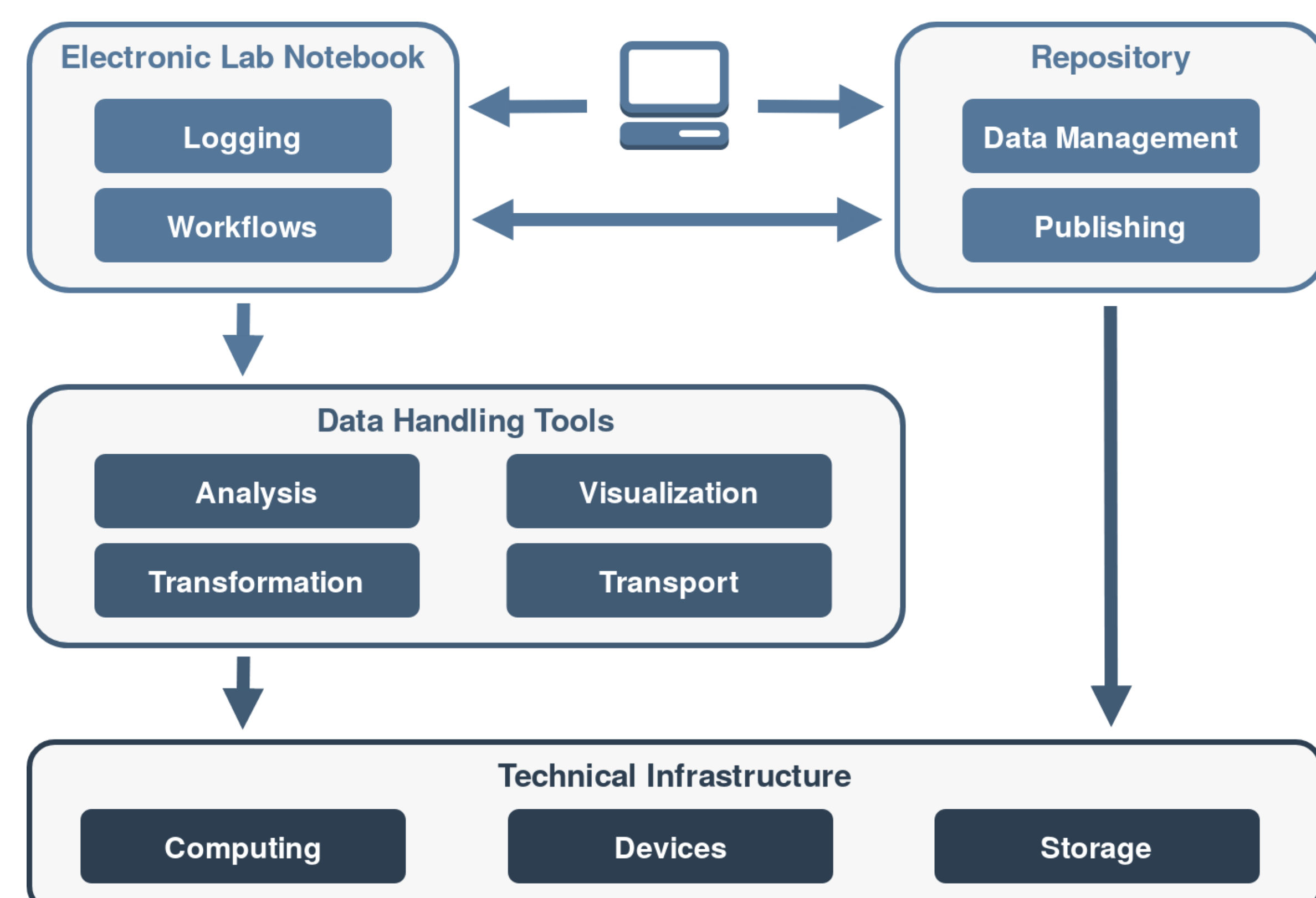


1. Motivation

- In **materials science**, the understanding of new materials is becoming increasingly complex.
- Without suitable **data science methods**, it will no longer be possible to manage the constantly growing volumes of data from simulations and experiments.
- An important aspect of being able to perform corresponding data analyses and share the results is the structured storage of research data and corresponding metadata using a suitable **research data infrastructure**.

2. Concepts

- A modular architecture is being pursued for this research data infrastructure, combining the two components **repository** and **electronic laboratory notebook (ELN)**.



- In this way, a **virtual research environment** is created that facilitates collaboration between researchers.

3. Implementation

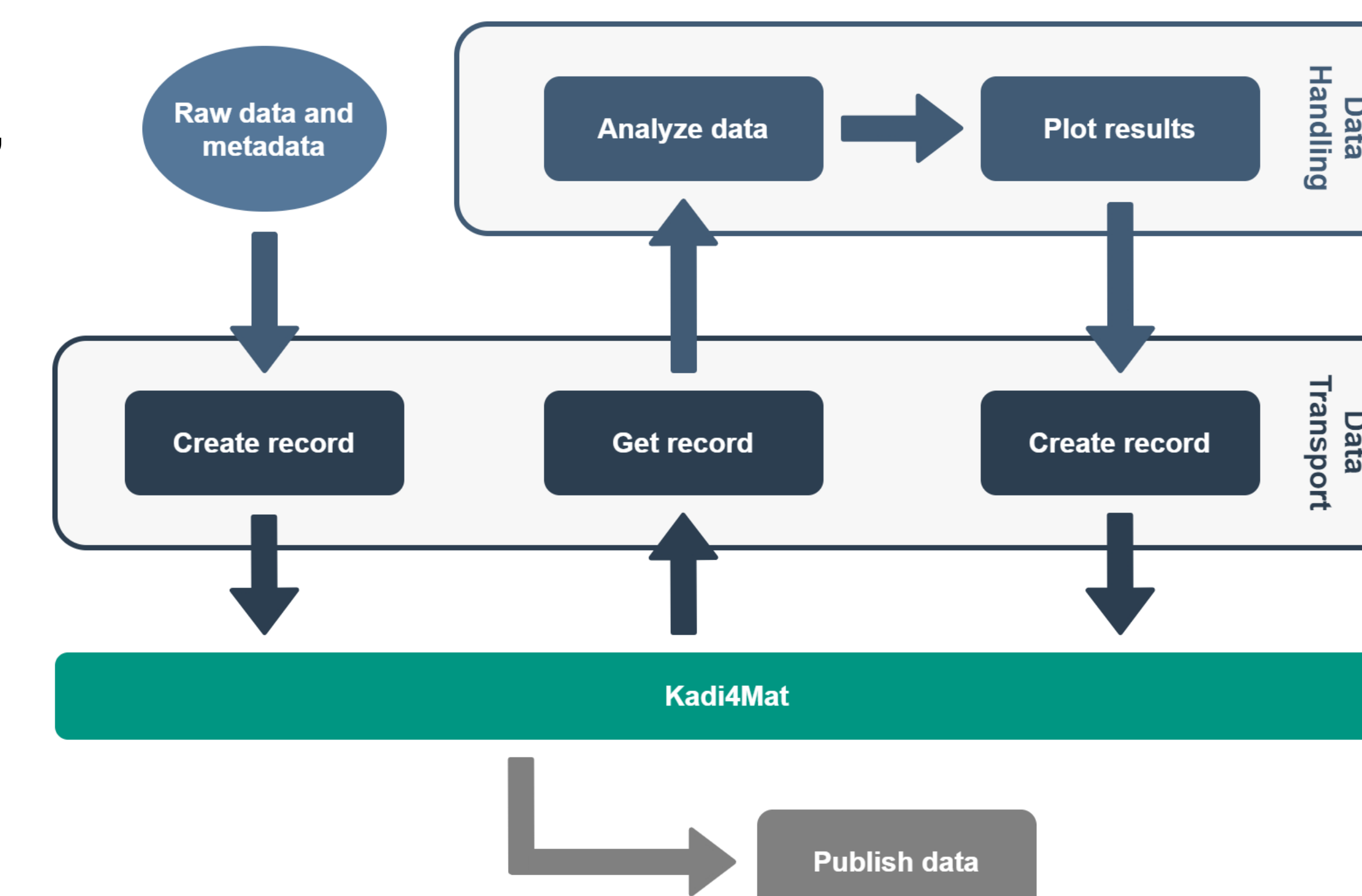


Karlsruhe Data Infrastructure
for Materials Science

- Kadi4Mat** [1] is an **open source** research data infrastructure which is being developed at the **KIT** in the context of several research projects.
- Multiple instances of the data infrastructure have already been deployed and show how structured data storage and data exchange are made possible.

4. Results

- Sharing of data within the own working group or with cooperation partners is easily possible by using the repository, while integrations are offered to directly publish data on external systems such as **Zenodo** or **RADAR** (*in progress*).
- A central part of the ELN component are the so called **workflows**, which each describe a number of steps using highly user- and application-specific tools that are executed in a well-defined order.
- Workflows offer a documented and reproducible way to automate different scientific steps, including running data handling or data transport tools, the latter enabling communication with a Kadi4Mat instance.



5. Conclusion

- Research data management with Kadi4Mat increases cooperation between researchers, taking into account the **FAIR data philosophy**.
- The future goal is to enable the electronic capture of the entire scientific workflow of daily research work.

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[1] Brandt, N., Griem, L., Herrmann, C., Schoof, E., Tosato, G., Zhao, Y., Zschumme, P. and Selzer, M., 2021. Kadi4Mat: A Research Data Infrastructure for Materials Science. *Data Science Journal*, 20(1), p.8. DOI: <http://doi.org/10.5334/dsj-2021-008>

