From FAIR Data to Knowledge and Novel Materials

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Research data paired with Artificial Intelligence (AI) enable of a new level of science. This particularly also holds for physics and materials research [1]. Here, the ultimate goal is to predict novel candidate materials for a given application, possibly even in regions of the materials space that no-one would think of. Our scientific vision is to build maps of material properties that will guide us in designing and finding new materials for a desired function. To reach this goal, the key prerequisites are novel AI tools with predictive power and Big Data – relevant and reliable data – all combined in a FAIR (Findable, Accessible, Interoperable, and Re-usable) data sharing platform. In 2014, the Novel Materials Discovery (NOMAD) Laboratory [2,3] set out to make this happen for computational materials science. For a real breakthrough, data from synthesis, experiment, and theory must be brought together. This is going to be realized in FAIRmat [4], the consortium representing condensed-matter physics and the chemical physics of solids within the German research data initiative (NFDI).

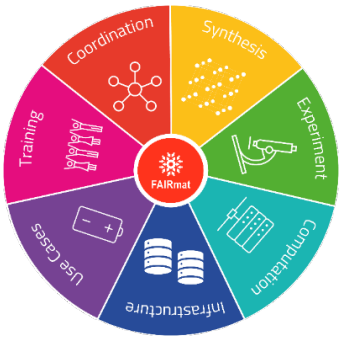

Fig. 1 Structure of the consortium FAIRmat.

References

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[2] C. Draxl and M. Scheffler, "NOMAD: The FAIR Concept for Big-Data-Driven Materials Science", MRS Bulletin **43**, 676 (2018).
[3] C. Draxl and M. Scheffler, "The NOMAD Laboratory: From Data Sharing to Artificial Intelligence", J. Phys. Mater. **2**, 036001 (2019).
[4] https://fair-di.eu/fairmat