An interdisciplinary approach to data management

Science Data Center für Molekulare Materialforschung

Patrick Altschuh[2], Stefan Bräse[1], Thomas Hartmann[3], Doris Jaeger[1], Nicole Jung[1], Arnd Koeppe[1], Peter Krauss[1], Carolin Leister[1], Britta Nestler[1], Gunther Schiefer[1], Clemens Schreiber[1], Michael Selzer[1], Martin Starman[1], Giovanna Tosato[1]

[1] Karlsruher Institut für Technologie; [2] Hochschule Karlsruhe; [3] FIZ Karlsruhe
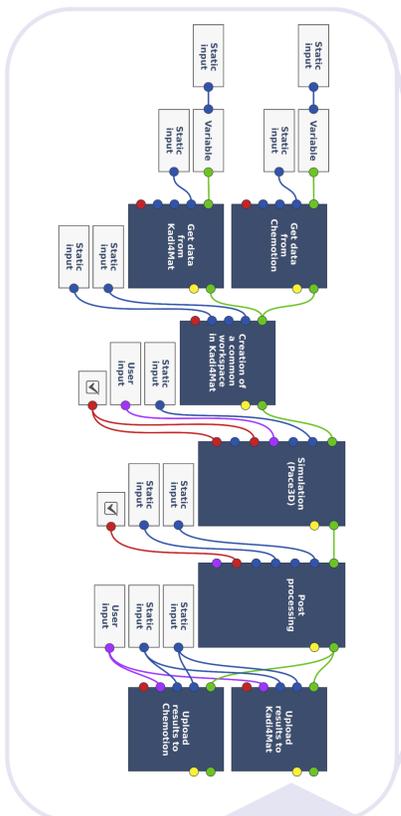
Concept

Many scientific issues involve interdisciplinary approaches that demand scientists with diverse skills and research fields. For the design and fabrication of new materials, this is especially true since new materials with macroscopically observable properties must be proposed based on changes at the molecular level. Research projects of this kind pose particular challenges for efficient execution and documentation, as research data management (RDM) tools usually fit very well to a specific research area, but cannot provide solutions for interdisciplinary topics. In order to guarantee consistent research and its documentation across disciplines, different tools, which may be used in several groups, must be used cooperatively.

The strategies developed in the context of the Science Data Center MoMaF enable research data management across scales. The RDM tools used for this are Chemotion and Kadi4Mat. The systems cover research at the molecular level (Chemotion ELN) as well as simulation activities on the meso- and macroscopic scale (Kadi4Mat), and will be extended within the Science Data Center to enable cooperative use of the systems for work across scales.
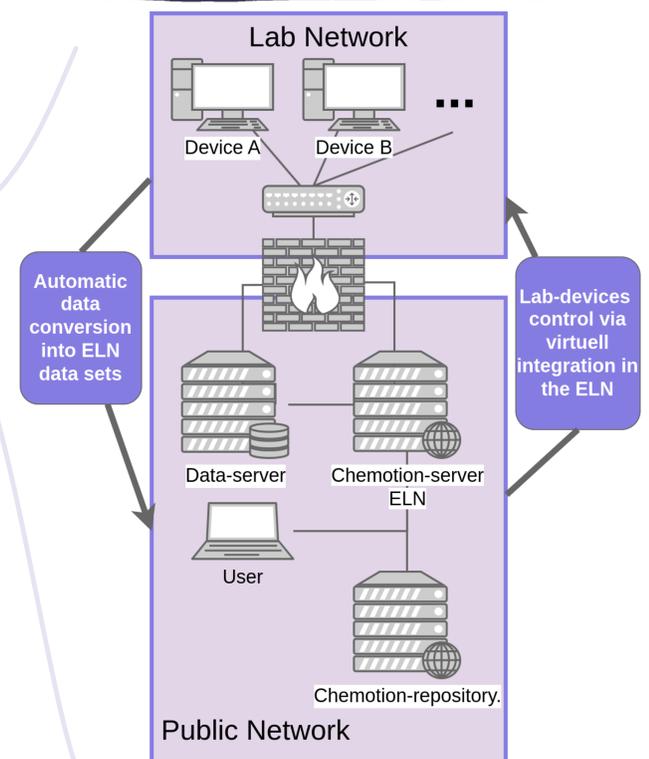
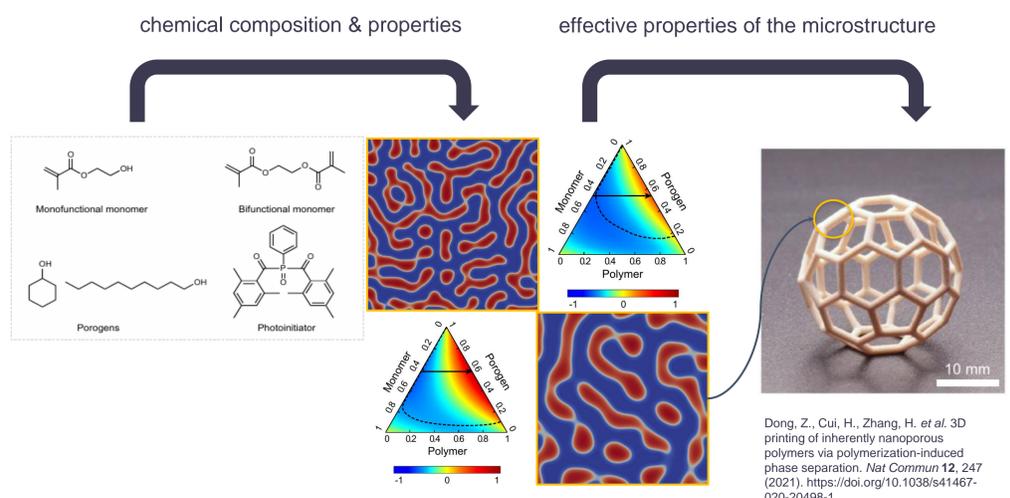## RDM Tools

Chemotion setup

Use case

A first use case shows how Chemotion ELN can be used to document necessary parameters at the molecular level, in order to then be able to manage simulations of phase separation processes on their basis in a further step with the help of Kadi4Mat. For this purpose, the procedure and documentation method of already completed projects were first analysed in order to be able to propose a concept for future proesses. Chemotion ELN is used in the presented procedure to document molecular descriptions, the performance of polymerization reactions and their outcome, as well as the properties obtained experimentally and from the literature. Kadi4Mat manages and transfers the parameters from the molecular description as input for mesoscopic simulations that describe the phase separation process in a time-dependent manner. Finally, by applying analysis tools on the time-dependent data via Kadi4Mat, macroscopic properties can be derived across scales as a function of the molecular composition.

Molecular level >>>>>>>> **Macroscopic scale**

Goal: Cooperative use for work across scales

chemical composition & properties

effective properties of the microstructure

Dong, Z., Cui, H., Zhang, H. et al. 3D printing of inherently nanoporous polymers via polymerization-induced phase separation. Nat Commun 12, 247 (2021). https://doi.org/10.1038/s41467-020-20498-1