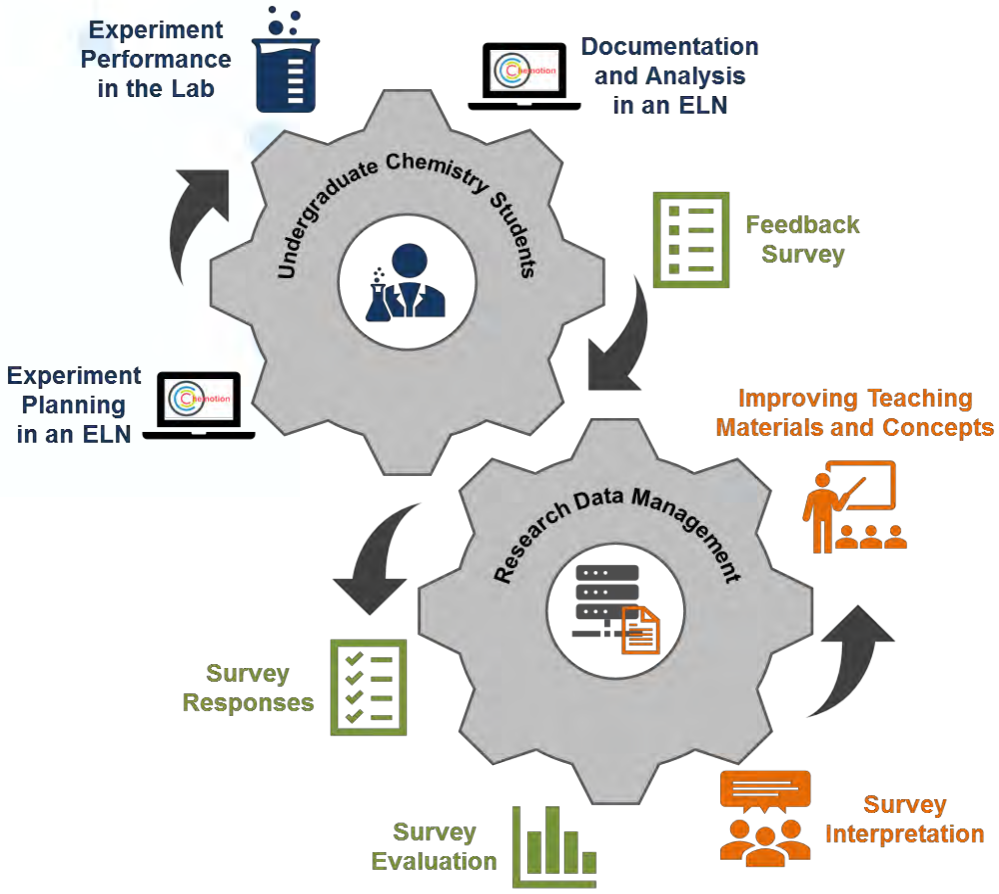
IAC Chair of Bioinorganic Chemistry | RWTH AACHEN UNIVERSITY

NFDI4Chem

ENHANCE YOUR DATA.

How to initiate the cultural change towards digital chemistry



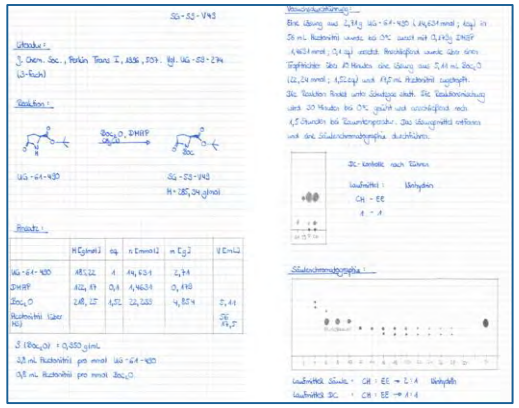
Prof. Dr. Sonja Herres-Pawlis

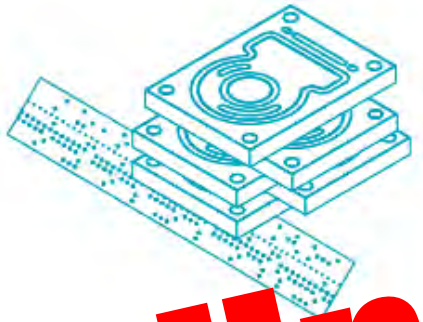
7th december 2023

Status Quo

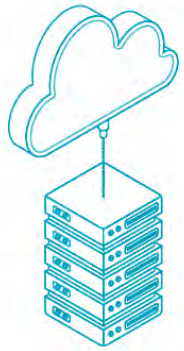
70 % still non-digital

Analogue / Digital



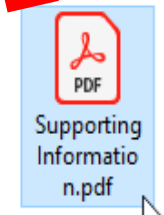


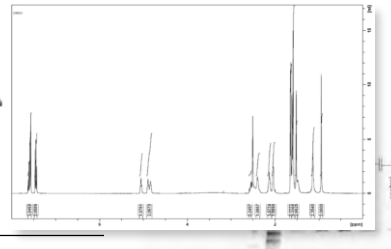
Digital

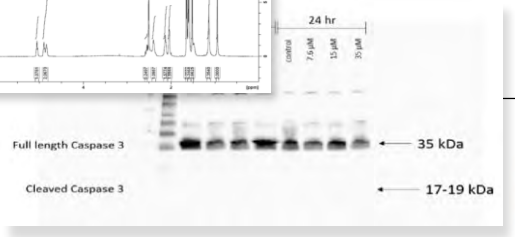


UnFAIR

Findable
Accessible
Interoperable
Reusable



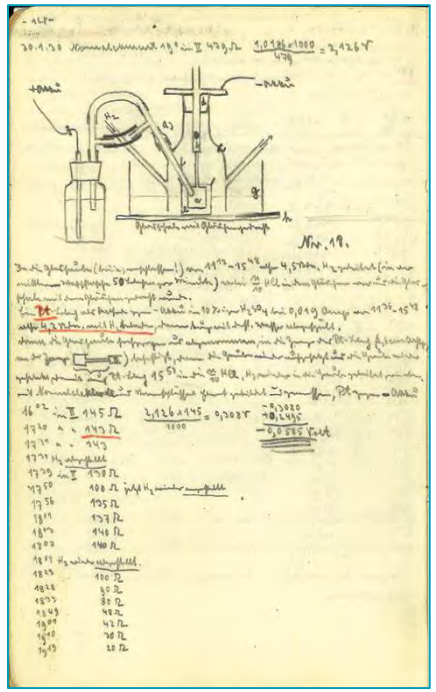




Not machine readable

Our Vision

1927



Digitalisation

Standards

Community

Experiment & Data collection

Data processing

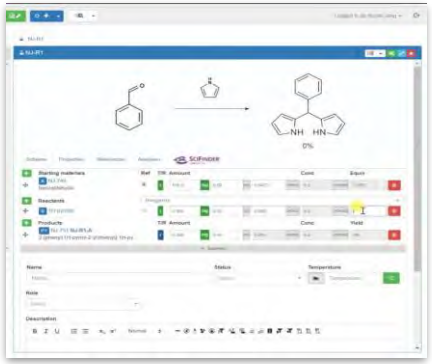
Data Analysis

Data preserved

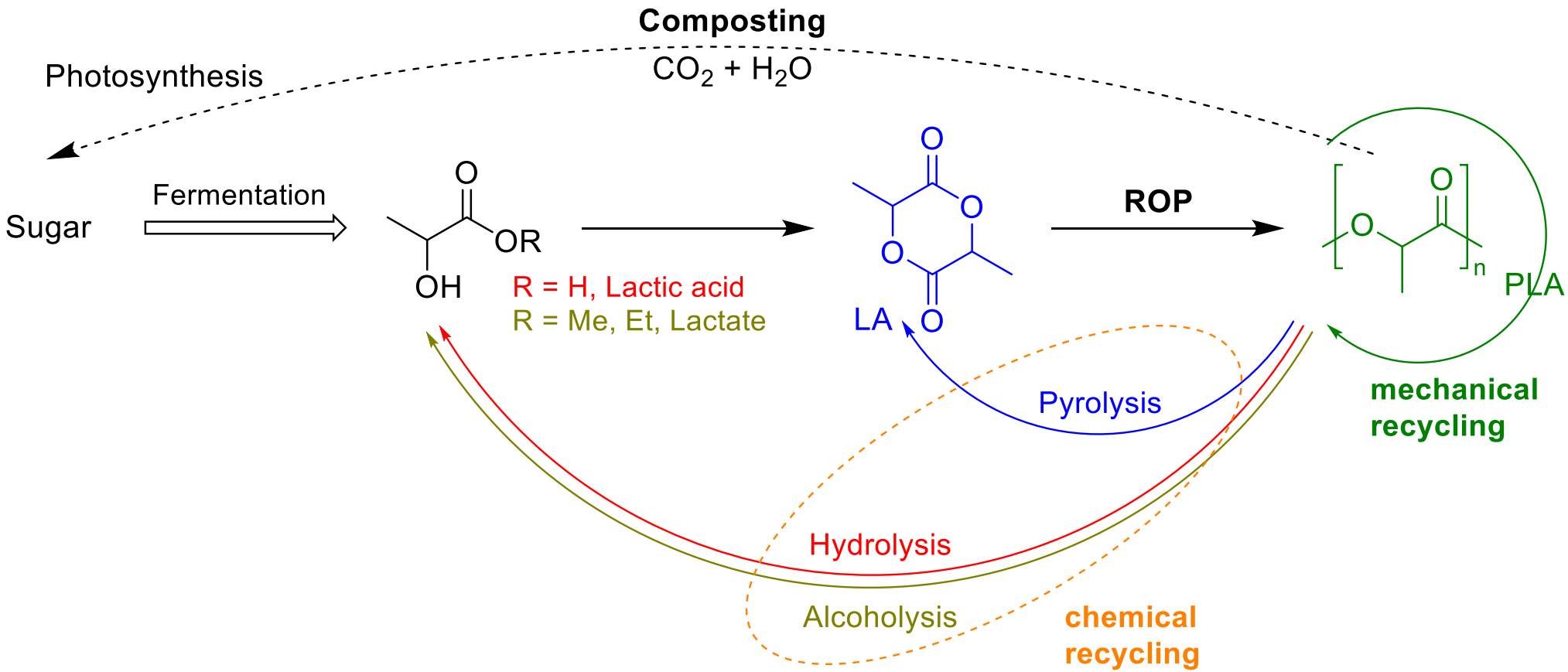
Data publication

Data re-use

FAIR DATA

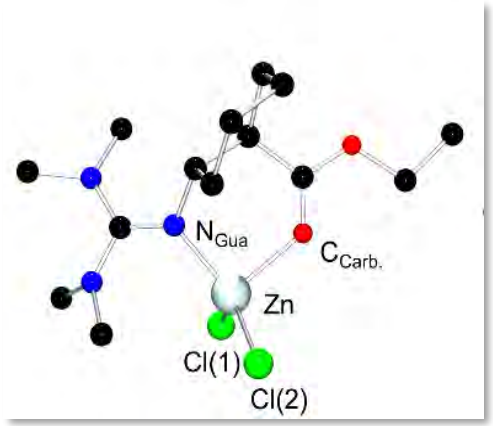


Polymerization and Depolymerization with one Catalyst



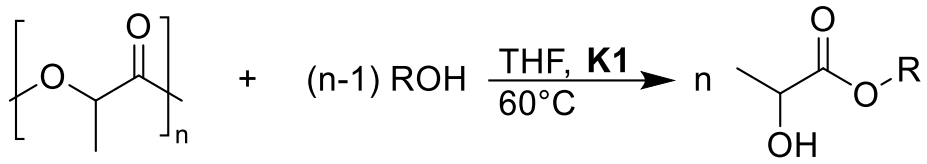
P. McKeown, M. D. Jones, *Sustain. Chem.* **2020**, *1*, 1–22.

Fractionated Recycling



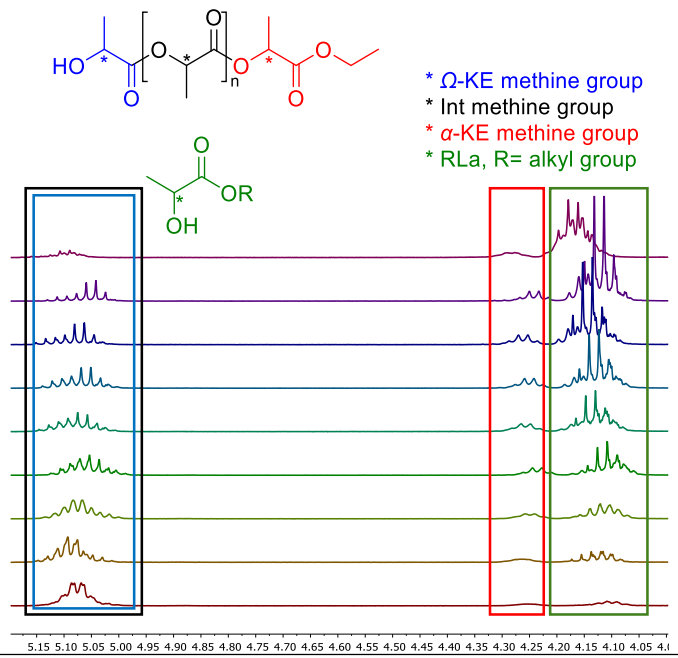
Depolymerisation of Bioplastics

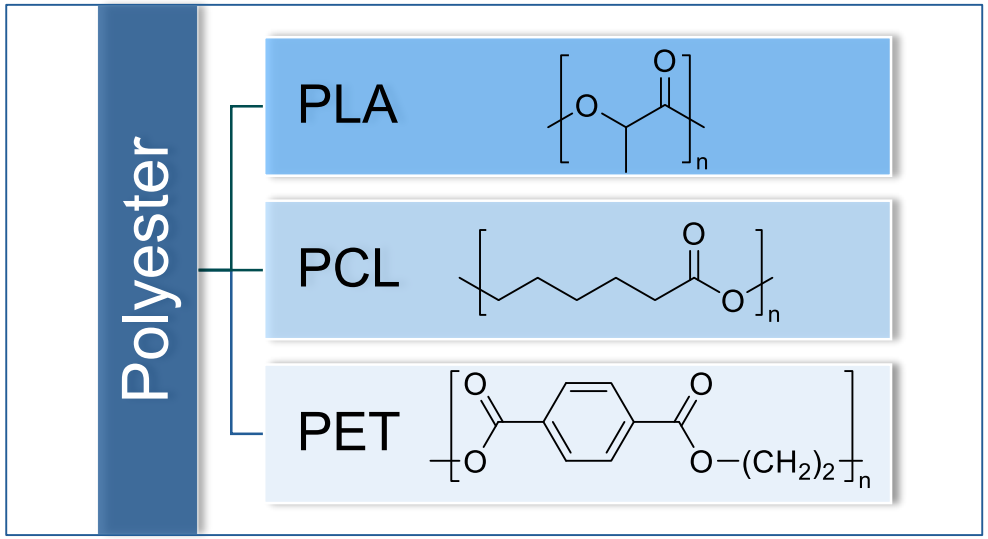
Reaction equation of the alcoholysis in solution:



Alcohol examples

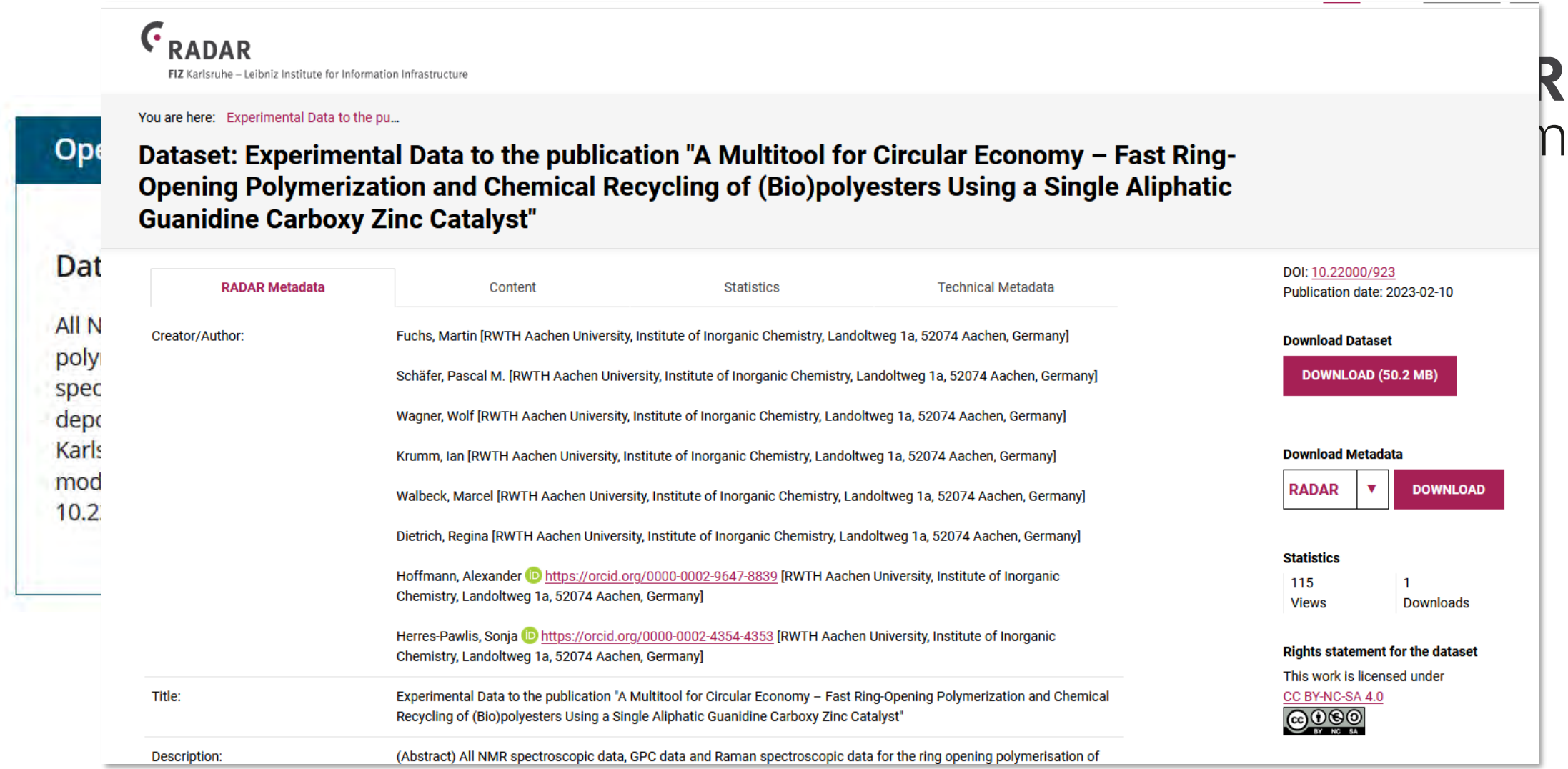
methanol
n-butanol
ethanol
i-butanol
benzyl alcohol
ethylene glycol
…





Just online: https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/cssc.202300192

FAIR Data: How to deposit data in a sustainable way: RADAR4Chem



RADAR
FIZ Karlsruhe – Leibniz Institute for Information Infrastructure

You are here: Experimental Data to the pu...

Dataset: Experimental Data to the publication "A Multitool for Circular Economy – Fast Ring-Opening Polymerization and Chemical Recycling of (Bio)polyesters Using a Single Aliphatic Guanidine Carboxy Zinc Catalyst"

RADAR Metadata | Content | Statistics | Technical Metadata

Creator/Author:	Fuchs, Martin [RWTH Aachen University, Institute of Inorganic Chemistry, Landoltweg 1a, 52074 Aachen, Germany] Schäfer, Pascal M. [RWTH Aachen University, Institute of Inorganic Chemistry, Landoltweg 1a, 52074 Aachen, Germany] Wagner, Wolf [RWTH Aachen University, Institute of Inorganic Chemistry, Landoltweg 1a, 52074 Aachen, Germany] Krumm, Ian [RWTH Aachen University, Institute of Inorganic Chemistry, Landoltweg 1a, 52074 Aachen, Germany] Walbeck, Marcel [RWTH Aachen University, Institute of Inorganic Chemistry, Landoltweg 1a, 52074 Aachen, Germany] Dietrich, Regina [RWTH Aachen University, Institute of Inorganic Chemistry, Landoltweg 1a, 52074 Aachen, Germany] Hoffmann, Alexander https://orcid.org/0000-0002-9647-8839 [RWTH Aachen University, Institute of Inorganic Chemistry, Landoltweg 1a, 52074 Aachen, Germany] Herres-Pawlis, Sonja https://orcid.org/0000-0002-4354-4353 [RWTH Aachen University, Institute of Inorganic Chemistry, Landoltweg 1a, 52074 Aachen, Germany]
Title:	Experimental Data to the publication "A Multitool for Circular Economy – Fast Ring-Opening Polymerization and Chemical Recycling of (Bio)polyesters Using a Single Aliphatic Guanidine Carboxy Zinc Catalyst"
Description:	(Abstract) All NMR spectroscopic data, GPC data and Raman spectroscopic data for the ring opening polymerisation of

DOI: 10.22000/923
Publication date: 2023-02-10

Download Dataset
DOWNLOAD (50.2 MB)

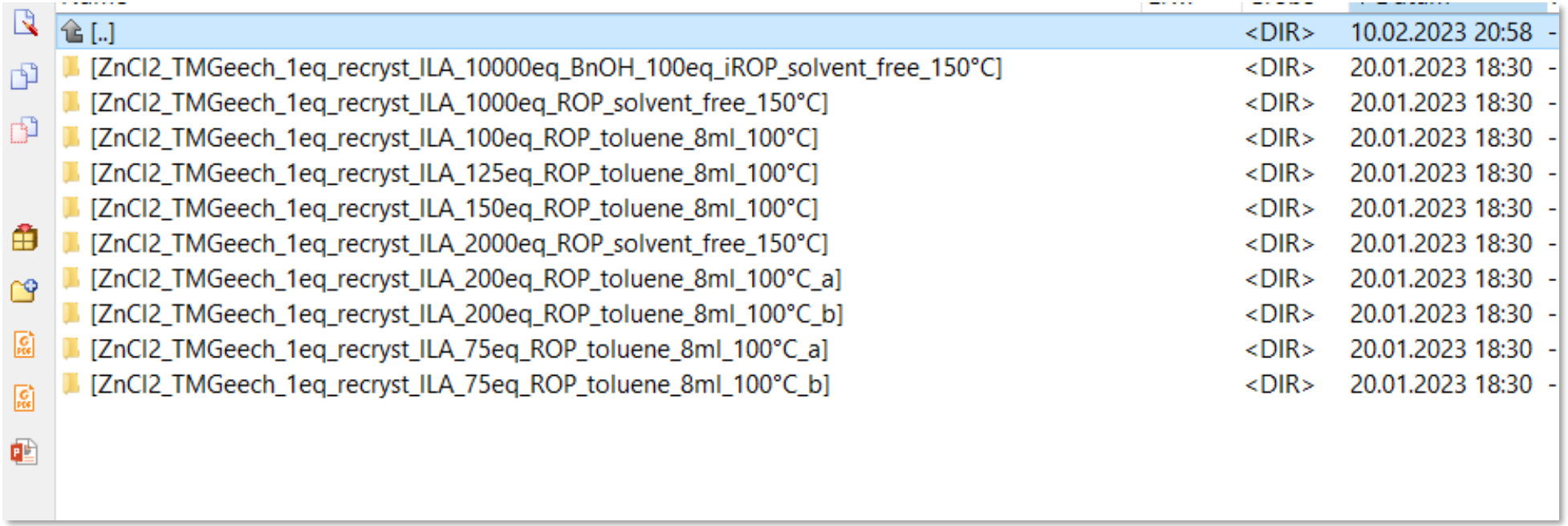
Download Metadata
RADAR ▼ DOWNLOAD

Statistics
115 Views | 1 Downloads

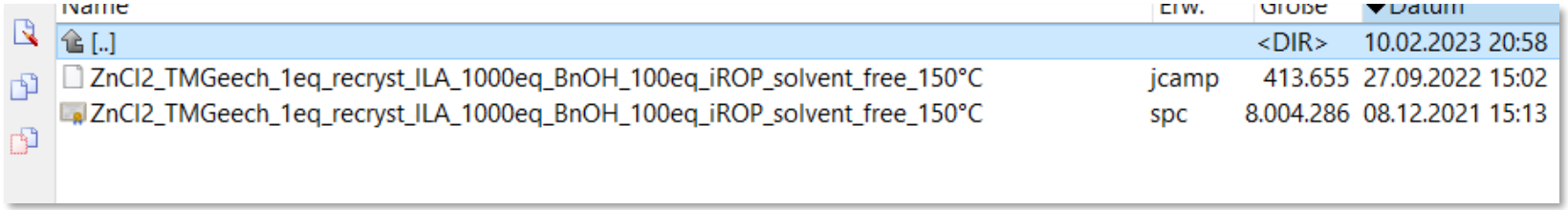
Rights statement for the dataset
This work is licensed under CC BY-NC-SA 4.0

Just online: https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/cssc.202300192

FAIR Data: How to deposit data in a sustainable way: RADAR4Chem



[..]	<DIR>	10.02.2023 20:58	-
[ZnCl2_TMGeech_1eq_recryst_ILA_10000eq_BnOH_100eq_iROP_solvent_free_150°C]	<DIR>	20.01.2023 18:30	-
[ZnCl2_TMGeech_1eq_recryst_ILA_1000eq_ROP_solvent_free_150°C]	<DIR>	20.01.2023 18:30	-
[ZnCl2_TMGeech_1eq_recryst_ILA_100eq_ROP_toluene_8ml_100°C]	<DIR>	20.01.2023 18:30	-
[ZnCl2_TMGeech_1eq_recryst_ILA_125eq_ROP_toluene_8ml_100°C]	<DIR>	20.01.2023 18:30	-
[ZnCl2_TMGeech_1eq_recryst_ILA_150eq_ROP_toluene_8ml_100°C]	<DIR>	20.01.2023 18:30	-
[ZnCl2_TMGeech_1eq_recryst_ILA_2000eq_ROP_solvent_free_150°C]	<DIR>	20.01.2023 18:30	-
[ZnCl2_TMGeech_1eq_recryst_ILA_200eq_ROP_toluene_8ml_100°C_a]	<DIR>	20.01.2023 18:30	-
[ZnCl2_TMGeech_1eq_recryst_ILA_200eq_ROP_toluene_8ml_100°C_b]	<DIR>	20.01.2023 18:30	-
[ZnCl2_TMGeech_1eq_recryst_ILA_75eq_ROP_toluene_8ml_100°C_a]	<DIR>	20.01.2023 18:30	-
[ZnCl2_TMGeech_1eq_recryst_ILA_75eq_ROP_toluene_8ml_100°C_b]	<DIR>	20.01.2023 18:30	-



Name	Erw.	Größe	Datum
[..]		<DIR>	10.02.2023 20:58
ZnCl2_TMGeech_1eq_recryst_ILA_1000eq_BnOH_100eq_iROP_solvent_free_150°C	jcamp	413.655	27.09.2022 15:02
ZnCl2_TMGeech_1eq_recryst_ILA_1000eq_BnOH_100eq_iROP_solvent_free_150°C	spc	8.004.286	08.12.2021 15:13

Just online: https://chemistry-europe.onlinelibrary.wiley.com/doi/10.1002/cssc.202300192

Integration into Curricular Teaching

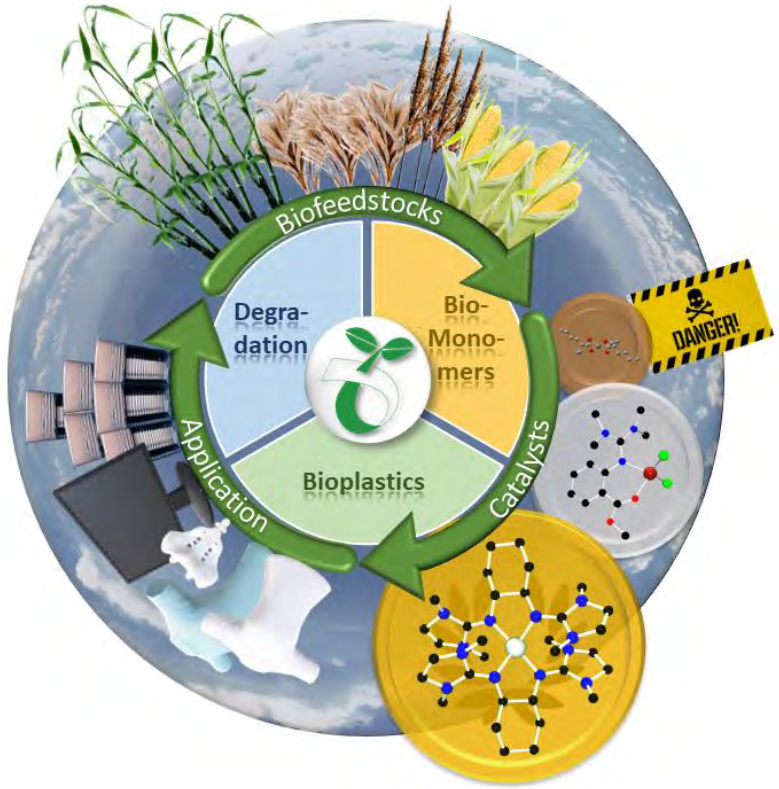
More direct and faster by hidden integration:

Example: in a Master lecture

Master lecture (2h per week) in the free area of the

Master studies @RWTH

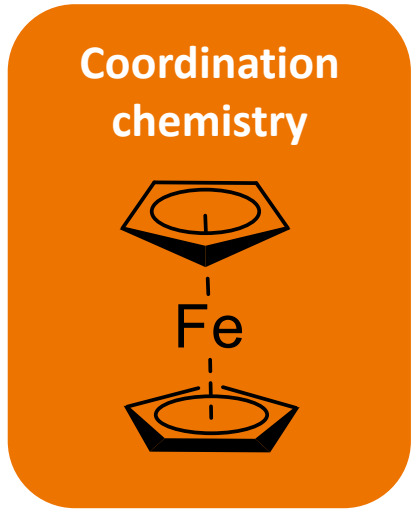
- Sustainable coordinative polymerisation catalysis
- 80-100 students, 50 take the exam
- Explaining chemistry with case studies
- Dissecting the RDM of the case studies (good and bad examples)
- Integrating videos on the basics of RDM from RWTH library/NFDI4Chem



Teaching the next generation

Advanced inorganic lab course for undergraduate students

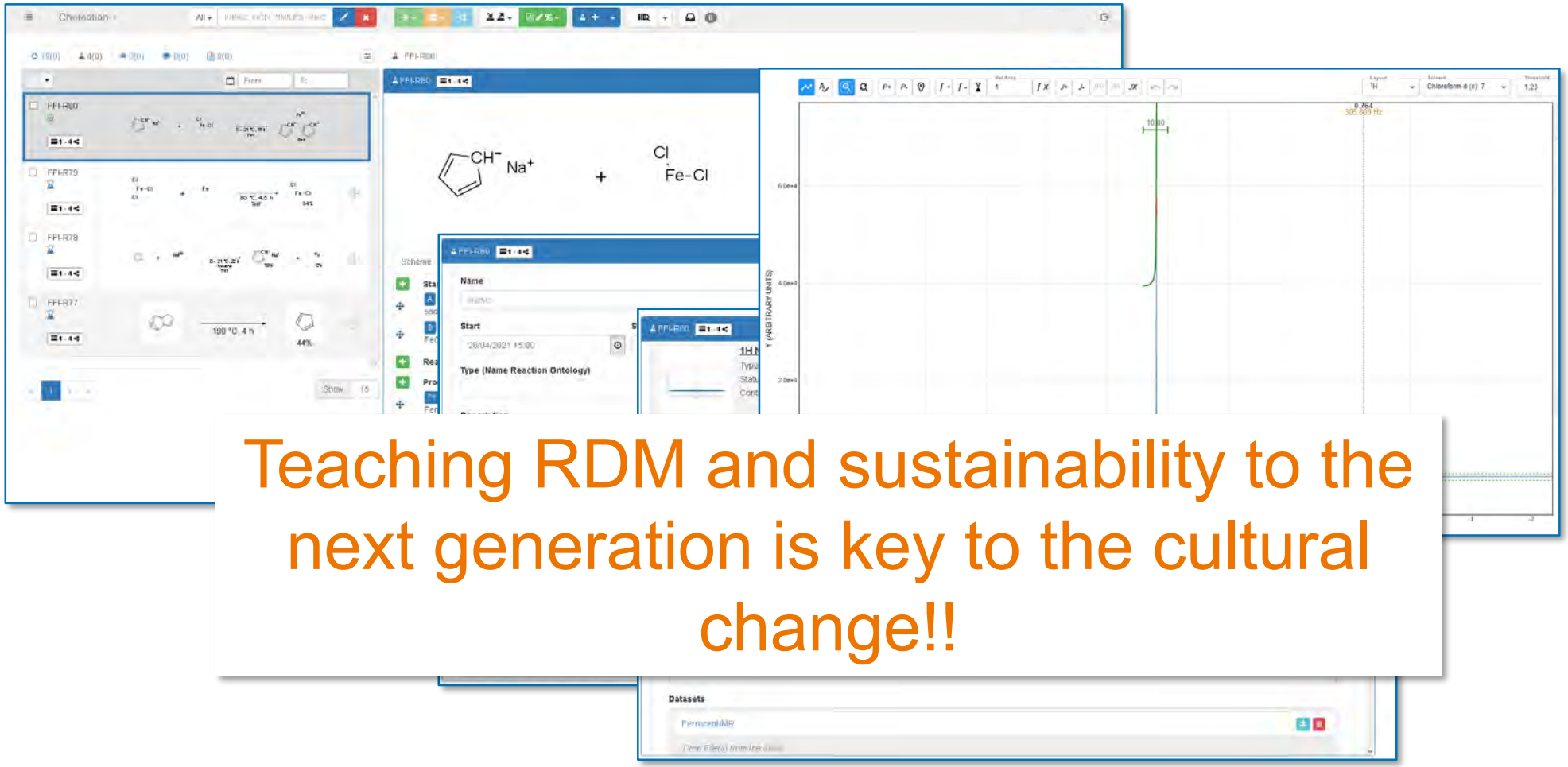
- Mandatory lab course for 5th semester bachelor students at RWTH Aachen
- Each winter term: 3 thematic blocks, 110 – 120 students
- Implementation of the Chemotion ELN (since WT20/21):
  - Synthesis of Ferrocene in the lab
  - Complete processing (planning, documentation, analysis) in the Chemotion ELN
- Learning unit on research data management (since WT20/21):
  - Short videos on the basics of RDM, FAIR principles, data management plans, metadata, and InChI & SMILES
  - Final test on RDM which students must pass in order to pass the lab course



Chemotion

Digital Documentation in the ELN

Processing of the synthesis of Ferrocene in the Chemotion ELN



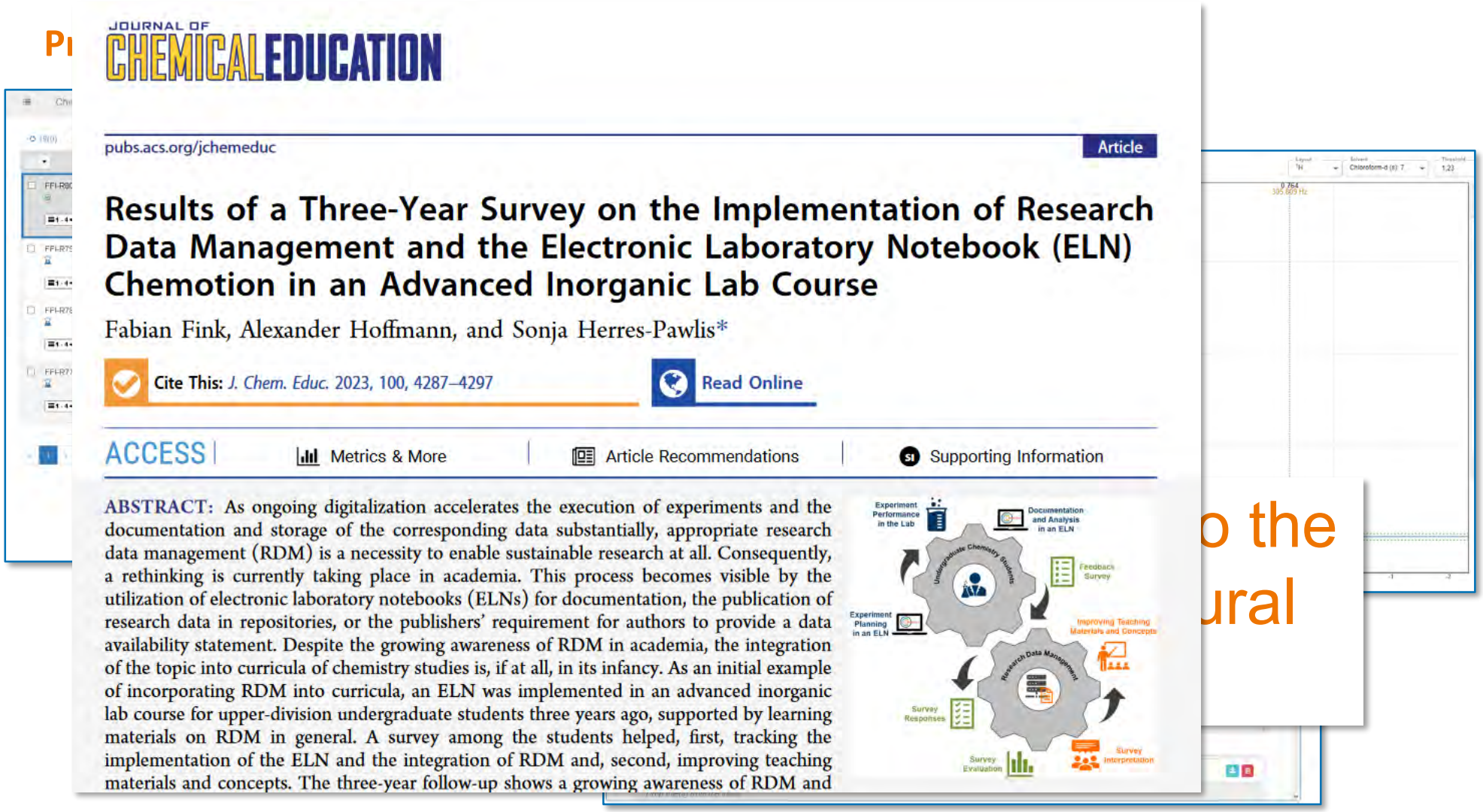
Teaching RDM and sustainability to the next generation is key to the cultural change!!

ELN videos on YouTube

Chemotion

10

Teaching the next generation



JOURNAL OF CHEMICAL EDUCATION

pubs.acs.org/jchemeduc

Article

Results of a Three-Year Survey on the Implementation of Research Data Management and the Electronic Laboratory Notebook (ELN) Chemotion in an Advanced Inorganic Lab Course

Fabian Fink, Alexander Hoffmann, and Sonja Herres-Pawlis*

Cite This: *J. Chem. Educ.* 2023, 100, 4287–4297

Read Online

ACCESS | Metrics & More | Article Recommendations | Supporting Information

ABSTRACT: As ongoing digitalization accelerates the execution of experiments and the documentation and storage of the corresponding data substantially, appropriate research data management (RDM) is a necessity to enable sustainable research at all. Consequently, a rethinking is currently taking place in academia. This process becomes visible by the utilization of electronic laboratory notebooks (ELNs) for documentation, the publication of research data in repositories, or the publishers' requirement for authors to provide a data availability statement. Despite the growing awareness of RDM in academia, the integration of the topic into curricula of chemistry studies is, if at all, in its infancy. As an initial example of incorporating RDM into curricula, an ELN was implemented in an advanced inorganic lab course for upper-division undergraduate students three years ago, supported by learning materials on RDM in general. A survey among the students helped, first, tracking the implementation of the ELN and the integration of RDM and, second, improving teaching materials and concepts. The three-year follow-up shows a growing awareness of RDM and

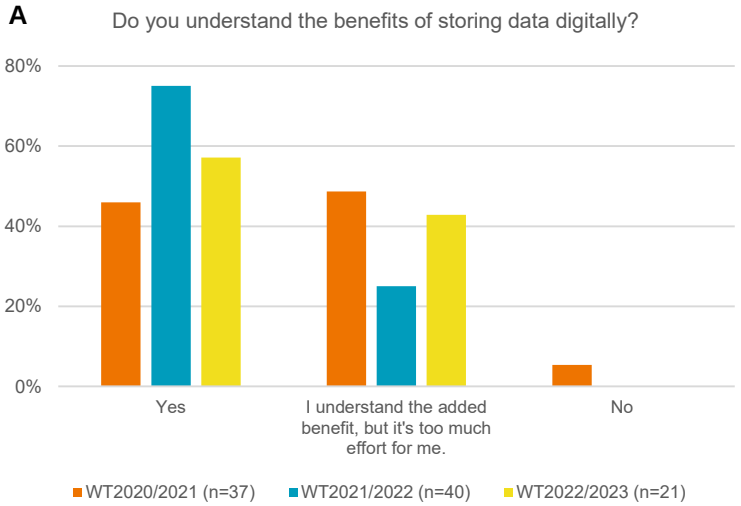
o the
ural

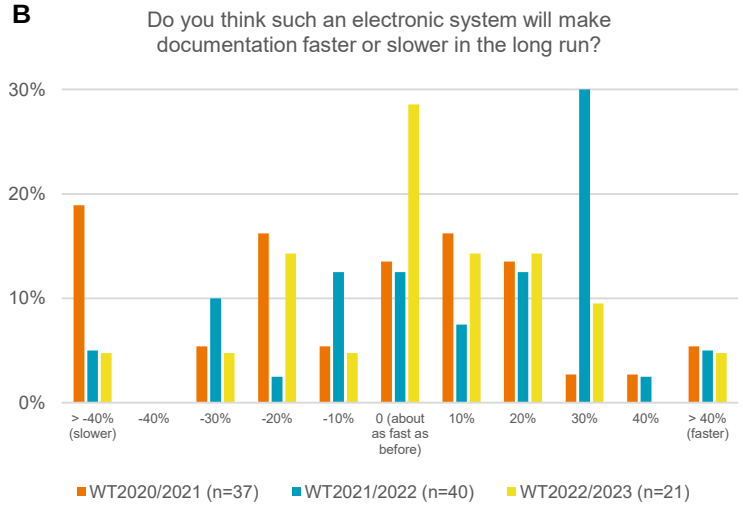
ELN videos
on YouTube

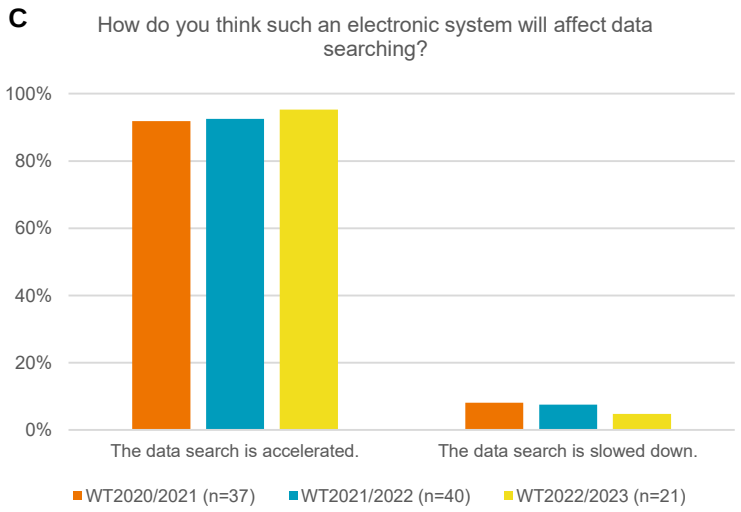
Chemotion

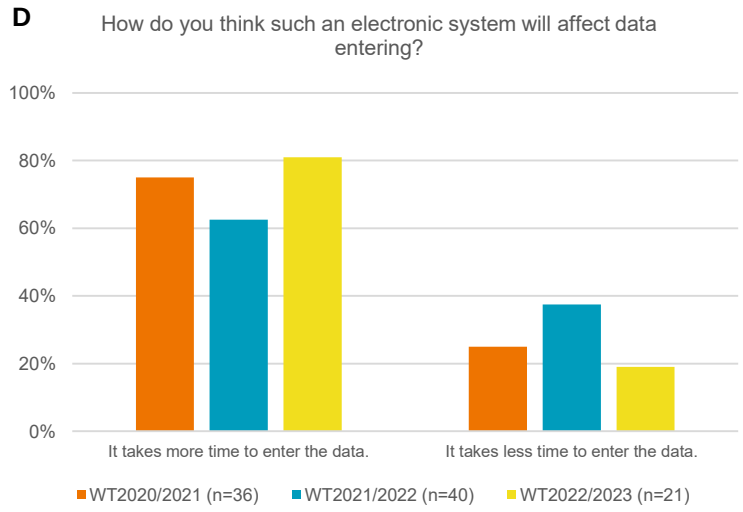
J. Chem. Educ. 2023, 100, 11, 4287–4297

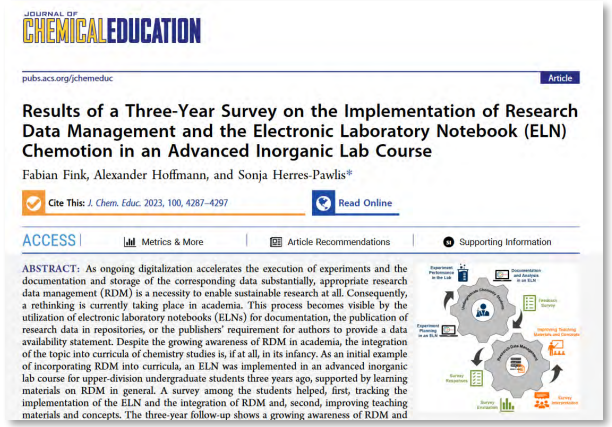
Teaching the next generation










JOURNAL OF CHEMICAL EDUCATION

pubs.acs.org/jchemeduc Article

Results of a Three-Year Survey on the Implementation of Research Data Management and the Electronic Laboratory Notebook (ELN) Chemotion in an Advanced Inorganic Lab Course

Fabian Fink, Alexander Hoffmann, and Sonja Herres-Pawlis*

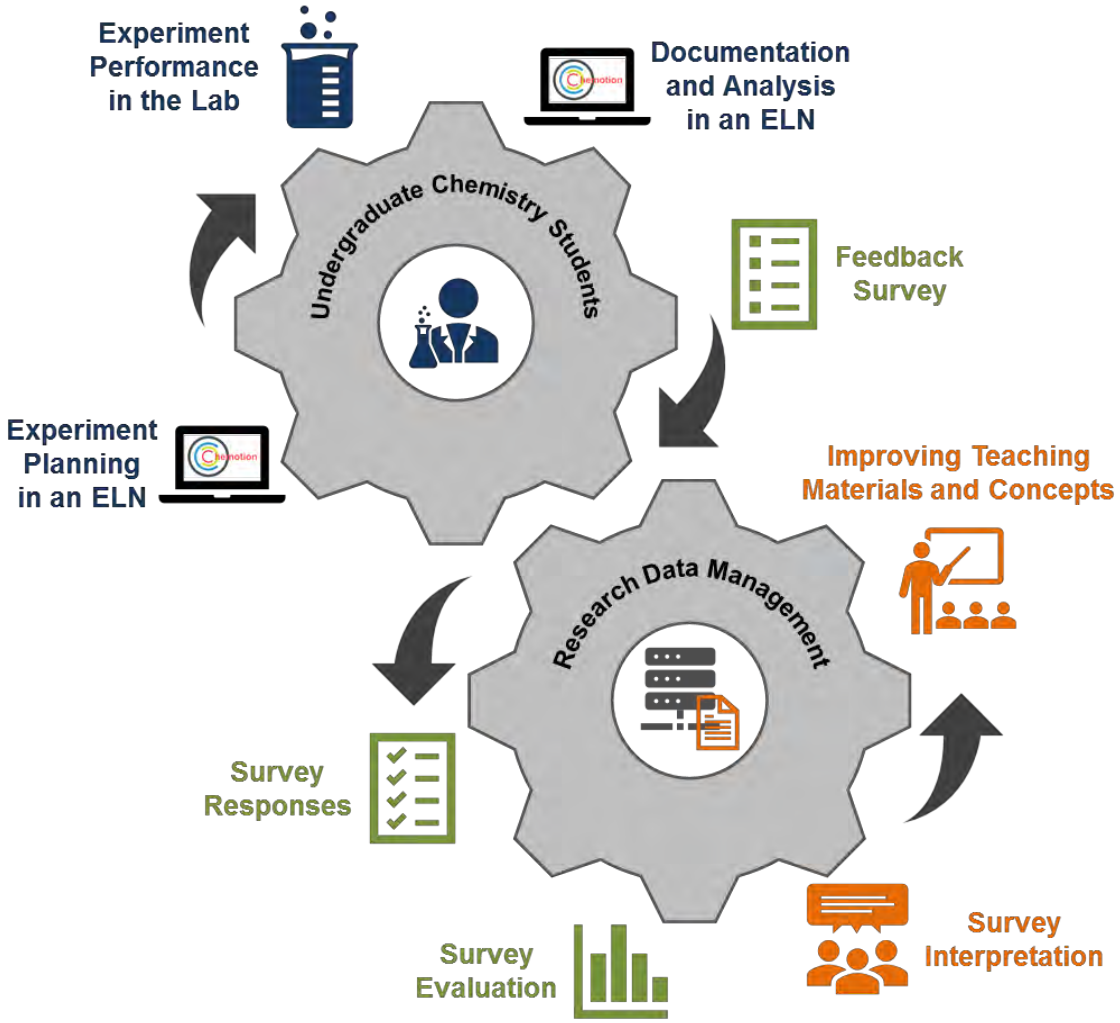
Cite This: *J. Chem. Educ.* 2023, 100, 4287–4297 Read Online

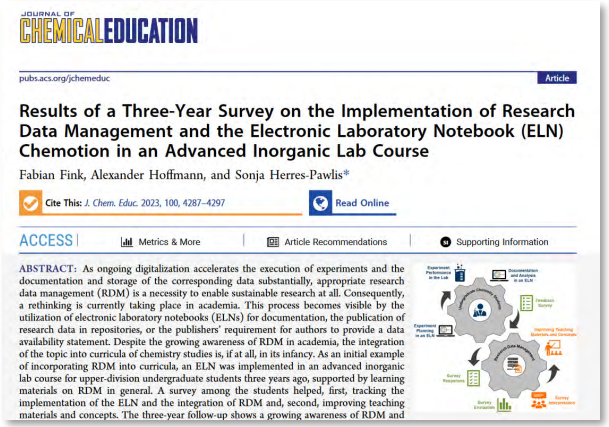
ACCESS | Metrics & More | Article Recommendations | Supporting Information

ABSTRACT: As ongoing digitalization accelerates the execution of experiments and the documentation and storage of the corresponding data substantially, appropriate research data management (RDM) is a necessity to enable sustainable research at all. Consequently, a rethinking is currently taking place in academia. This process becomes visible by the utilization of electronic laboratory notebooks (ELNs) for documentation, the publication of research data in repositories, or the publishers' requirement for authors to provide a data availability statement. Despite the growing awareness of RDM in academia, the integration of the topic into curricula of chemistry studies is, if at all, in its infancy. As an initial example of incorporating RDM into curricula, an ELN was implemented in an advanced inorganic lab course for upper-division undergraduate students three years ago, supported by learning materials on RDM in general. A survey among the students helped, first, tracking the implementation of the ELN and the integration of RDM and, second, improving teaching materials and concepts. The three-year follow-up shows a growing awareness of RDM and

J. Chem. Educ. 2023, 100, 11, 4287–4297

Teaching the next generation





JOURNAL OF CHEMICAL EDUCATION

pubs.acs.org/jchemeduc Article

Results of a Three-Year Survey on the Implementation of Research Data Management and the Electronic Laboratory Notebook (ELN) Chemotion in an Advanced Inorganic Lab Course

Fabian Fink, Alexander Hoffmann, and Sonja Herres-Pawlis*

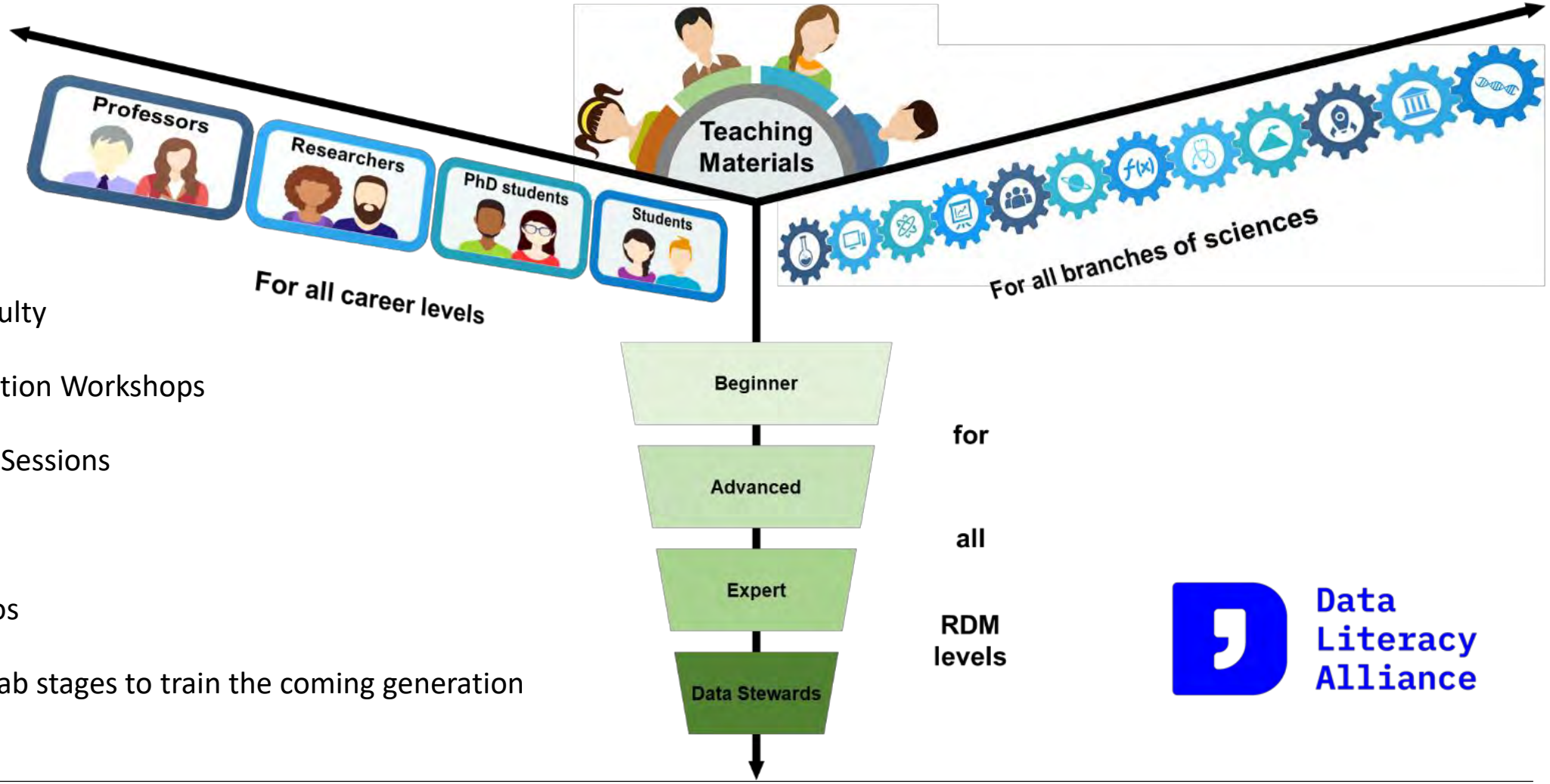
Cite This: *J. Chem. Educ.* 2023, 100, 4287–4297 Read Online

ACCESS | Metrics & More | Article Recommendations | Supporting Information

ABSTRACT: As ongoing digitalization accelerates the execution of experiments and the documentation and storage of the corresponding data substantially, appropriate research data management (RDM) is a necessity to enable sustainable research at all. Consequently, a rethinking is currently taking place in academia. This process becomes visible by the utilization of electronic laboratory notebooks (ELNs) for documentation, the publication of research data in repositories, or the publishers' requirement for authors to provide a data availability statement. Despite the growing awareness of RDM in academia, the integration of the topic into curricula of chemistry studies is, if at all, in its infancy. As an initial example of incorporating RDM into curricula, an ELN was implemented in an advanced inorganic lab course for upper-division undergraduate students three years ago, supported by learning materials on RDM in general. A survey among the students helped, first, tracking the implementation of the ELN and the integration of RDM and, second, improving teaching materials and concepts. The three-year follow-up shows a growing awareness of RDM and

J. Chem. Educ. 2023, 100, 11, 4287–4297

Dimensions of RDM teaching



- Materials for Faculty
- RDM and Chemotion Workshops
- Chemotion Q&A Sessions
- Best practices
- Chemotion Videos
- Integration into lab stages to train the coming generation

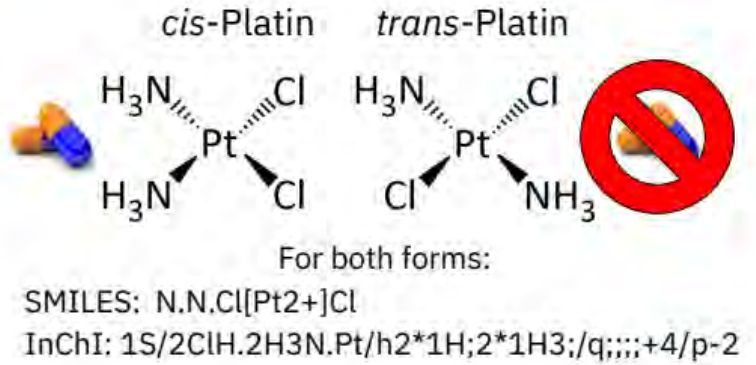
Data Literacy Alliance

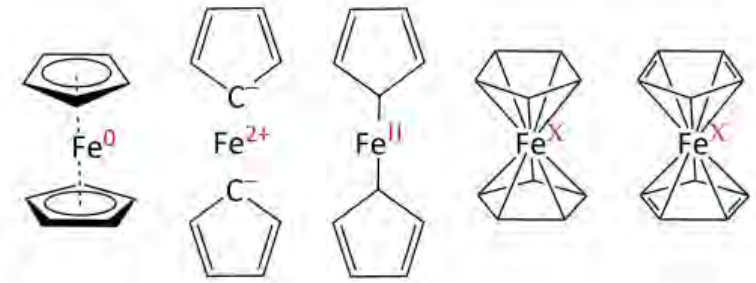
Concept: https://zenodo.org/record/6475541#.Y0G7QkzP1PY

14

InChI Participation

- Intensive involvement in InChI subcommittee on molecular inorganics and the Board of the InChI Trust
- Mind change on formal bond breaking of metal-donor bonds towards a non-disconnection approach
- Bringing the InChI to Machine Learning
- New InChI Version just out: v1.07 (https://github.com/IUPAC-InChI):
- Cleaned, faster, on GitHub available, community can contribute
- WebDemo: https://iupac-inchi.github.io/InChI-Web-Demo/





Acknowledgement

Dr. Alexander Hoffmann

Dr. Jochen Ortmeyer

Fabian Fink

Martin Fuchs

InChI:

Dr. Djordje Baljozovic

Jan Brammer

Frank Lange

Nauman Khan

Chemotion: Dr. Nicole Jung & Team

StructurePendium: Dr. Gerd Blanke

Data Literacy Alliance

BioSC Bioeconomy Science Center

GEFÖRDERT VOM Bundesministerium für Bildung und Forschung

TOTAL Corbion

DBU Deutsche Bundesstiftung Umwelt

FCI FONDS DER CHEMISCHEN INDUSTRIE

SFB 985

VolkswagenStiftung

Chemotion

NFDI4Chem

DFG