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TIB

NFDI4Chem - Nationale Forschungsdateninfrastruktur für Chemie

Dr. Johannes Hunold

open-access.net Workshop "Auf dem Weg zu mehr Open Access im Fach Chemie - Rolle der Bibliotheken", 30. Juni 2021

NFDI in General

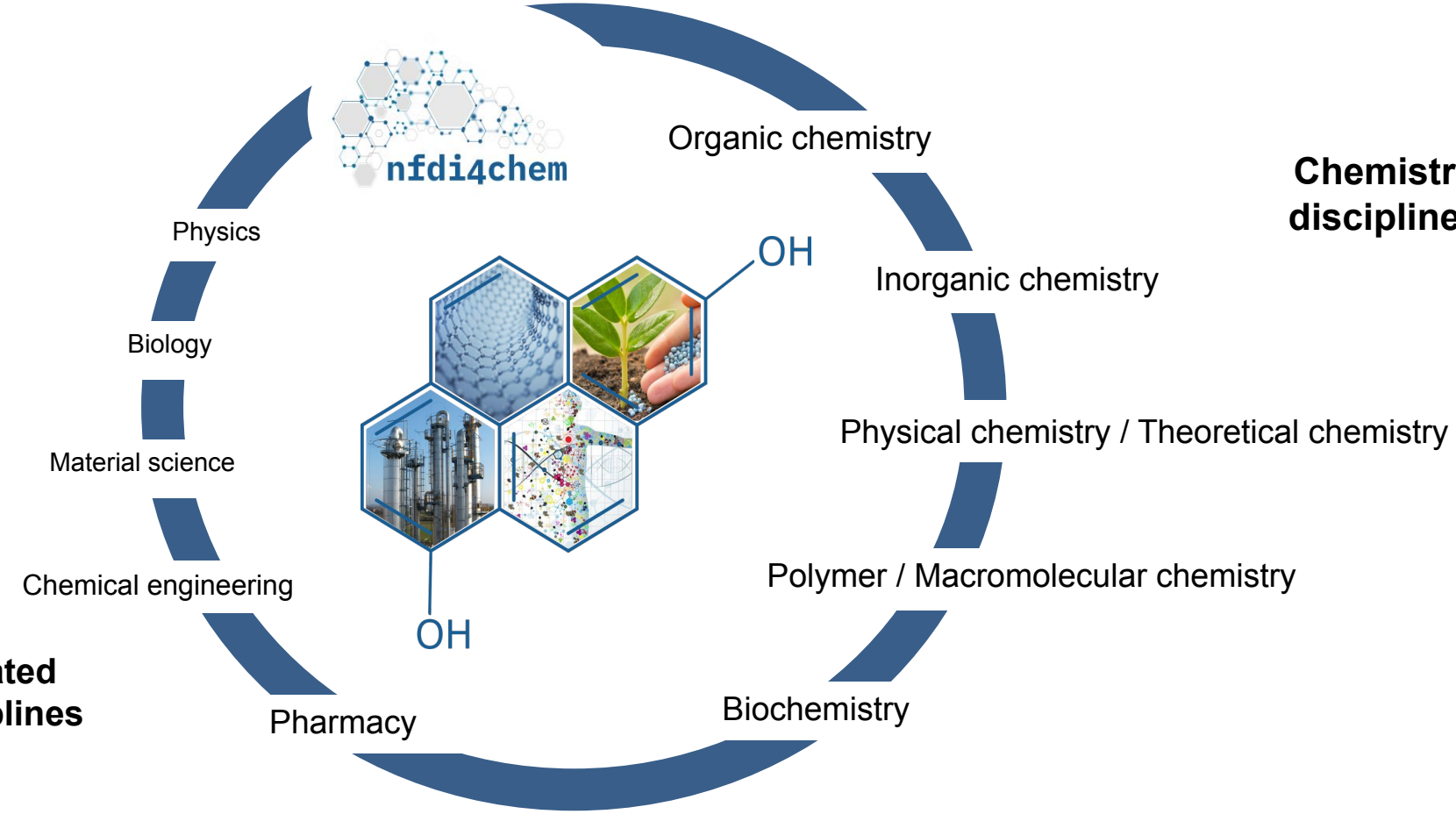
Federal Government and the 16 States decided to fund
a **N**ationale **F**orschungs**d**aten**i**nfrastruktur (NFDI) in Germany

- formal establishment of the NFDI association in October 2020
- providing up to 85 million € for a period of 10 years
- up to 30 consortia from all areas of science are funded
- self-organized & strictly science-driven process of close collaboration (not competing within the individual scientific fields)
- Aim: exploit the valuable potential of research data and make them **f**indable, **a**ccessible, **i**nterconnected and (**r**e)usable = FAIR

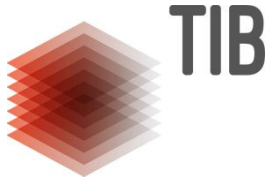
Explaining videos of DFG what is the NFDI (https://www.youtube.com/watch?v=x3Cvn1vNQ98&t=2s) & how is the review process (https://www.youtube.com/watch?v=XTzwPwMAqHM&t=1s)

NFDI4Chem - The Consortium for Chemistry

- consortium addresses the specific interests & needs of the chemical community



Who we are



technische universität dortmund

GEORG-AUGUST-UNIVERSITÄT GÖTTINGEN

KIT Karlsruher Institut für Technologie

chemotion

DPhG Deutsche Pharmazeutische Gesellschaft e.V.

GDCh Gesellschaft Deutscher Chemiker

Fritz-Haber-Institut

SCC Steinbuch Centre for Computing

FIZ Karlsruhe Leibniz-Institut für Informationsinfrastruktur

PTB Messen ▪ Forschen ▪ Wissen

BEILSTEIN INSTITUT

LMU

IPB Leibniz-Institut für Pflanzenbiochemie

RWTH AACHEN UNIVERSITY

JG|U Johannes Gutenberg Universität Mainz

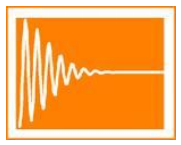
IDNMR

UFZ Helmholtz Centre for Environmental Research

CIC

Julius-Maximilians-Universität Würzburg

Technische Universität Braunschweig

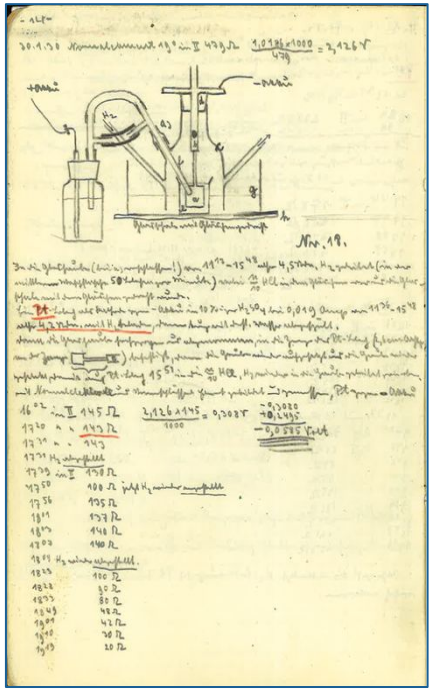


TECHNISCHE UNIVERSITÄT DRESDEN

DBG Deutsche Bunsen-Gesellschaft für physikalische Chemie e.V.

UNIVERSITÄT GREIFSWALD Wissen lockt. Seit 1456

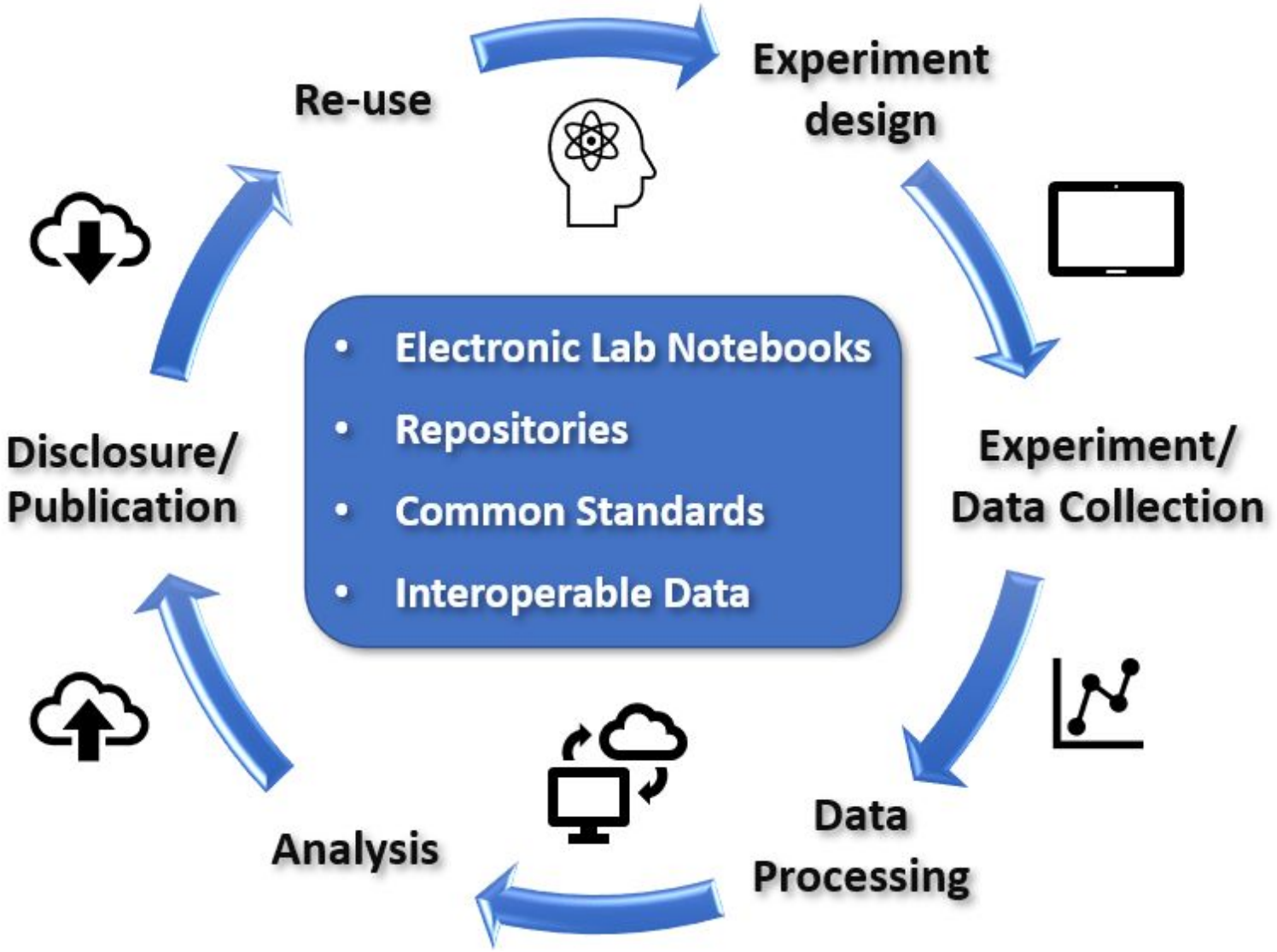
Our Vision



Digitalisation

Standards

Community

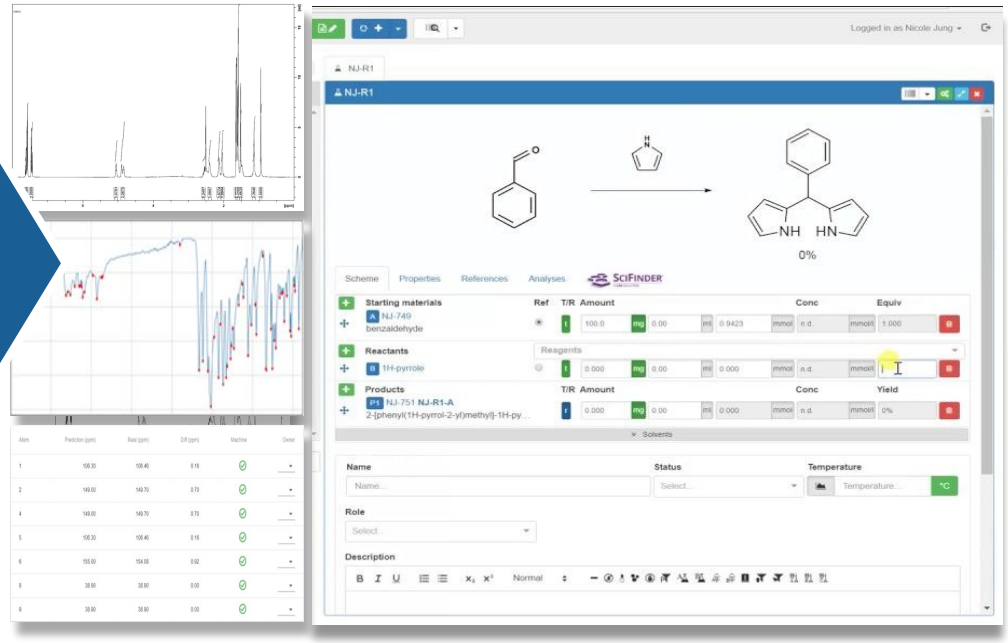


Smart Lab - Seamless Data Flows

Devices

Data

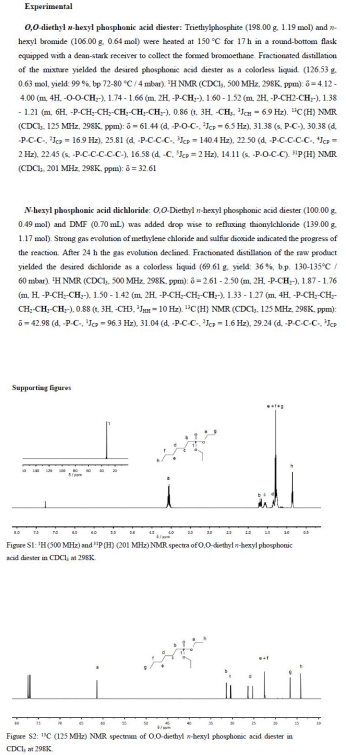
Electronic Lab Notebook (ELN)



Data

Generation of SI for "traditional" Paper Publication

Federated Repositories



Experimental

O,O-diethyl *n*-hexyl phosphonic acid diester: Triethylphosphite (198.00 g, 1.19 mol) and *n*-hexyl bromide (106.00 g, 0.64 mol) were heated at 150 °C for 17 h in a round-bottom flask equipped with a dean-stark receiver to collect the formed bromoethane. Fractionated distillation of the mixture yielded the desired phosphonic acid diester as a colorless liquid. (126.53 g, 0.63 mol, yield: 99 %, bp 72-80 °C / 4 mbar). ^{1}H NMR ($CDCl_3$, 500 MHz, 298K, ppm): δ = 4.12 - 4.00 (m, 4H, -O-O-CH_2-), 1.74 - 1.66 (m, 2H, -P-CH_2-), 1.60 - 1.52 (m, 2H, -P-$CH2$-CH_2-), 1.38 - 1.21 (m, 6H, -P-CH_2-CH_2-CH_2-CH_2-), 0.86 (t, 3H, -CH_3, $^{3}J_{CH}$ = 6.9 Hz). ^{13}C{H} NMR ($CDCl_3$, 125 MHz, 298K, ppm): δ = 61.44 (d, -P-O-C-, $^{2}J_{CP}$ = 6.5 Hz), 31.38 (s, P-C-), 30.38 (d, -P-C-C-, $^{3}J_{CP}$ = 16.9 Hz), 25.81 (d, -P-C-C-C-, $^{2}J_{CP}$ = 140.4 Hz), 22.50 (d, -P-C-C-C-C-, $^{4}J_{CP}$ = 2 Hz), 22.45 (s, -P-C-C-C-C-C-), 16.58 (d, -C-, $^{3}J_{CP}$ = 2 Hz), 14.11 (s, -P-O-C-C). ^{31}P{H} NMR ($CDCl_3$, 201 MHz, 298K, ppm): δ = 32.61

N-hexyl phosphonic acid dichloride: *O,O*-Diethyl *n*-hexyl phosphonic acid diester (100.00 g, 0.49 mol) and DMF (0.70 mL) was added drop wise to refluxing thionylchloride (139.00 g, 1.17 mol). Strong gas evolution of methylene chloride and sulfur dioxide indicated the progress of the reaction. After 24 h the gas evolution declined. Fractionated distillation of the raw product yielded the desired dichloride as a colorless liquid (69.61 g, yield: 36 %, b.p. 130-135°C / 60 mbar). ^{1}H NMR ($CDCl_3$, 500 MHz, 298K, ppm): δ = 2.61 - 2.50 (m, 2H, -P-CH_2-), 1.87 - 1.76 (m, H, -P-CH_2-CH_2-), 1.50 - 1.42 (m, 2H, -P-CH_2-CH_2-CH_2-), 1.33 - 1.27 (m, 4H, -P-CH_2-CH_2-CH_2-CH_2-CH_2-), 0.88 (t, 3H, -CH_3, $^{3}J_{HH}$ = 10 Hz). ^{13}C{H} NMR ($CDCl_3$, 125 MHz, 298K, ppm): δ = 42.98 (d, -P-C-, $^{1}J_{CP}$ = 96.3 Hz), 31.04 (d, -P-C-C-, $^{2}J_{CP}$ = 1.6 Hz), 29.24 (d, -P-C-C-C-, $^{3}J_{CP}$

Supporting figures

Figure S1: ^{1}H (500 MHz) and ^{31}P{H} (201 MHz) NMR spectra of O,O-diethyl *n*-hexyl phosphonic acid diester in $CDCl_3$ at 298K.

Figure S2: ^{13}C (125 MHz) NMR spectrum of O,O-diethyl *n*-hexyl phosphonic acid diester in $CDCl_3$ at 298K.

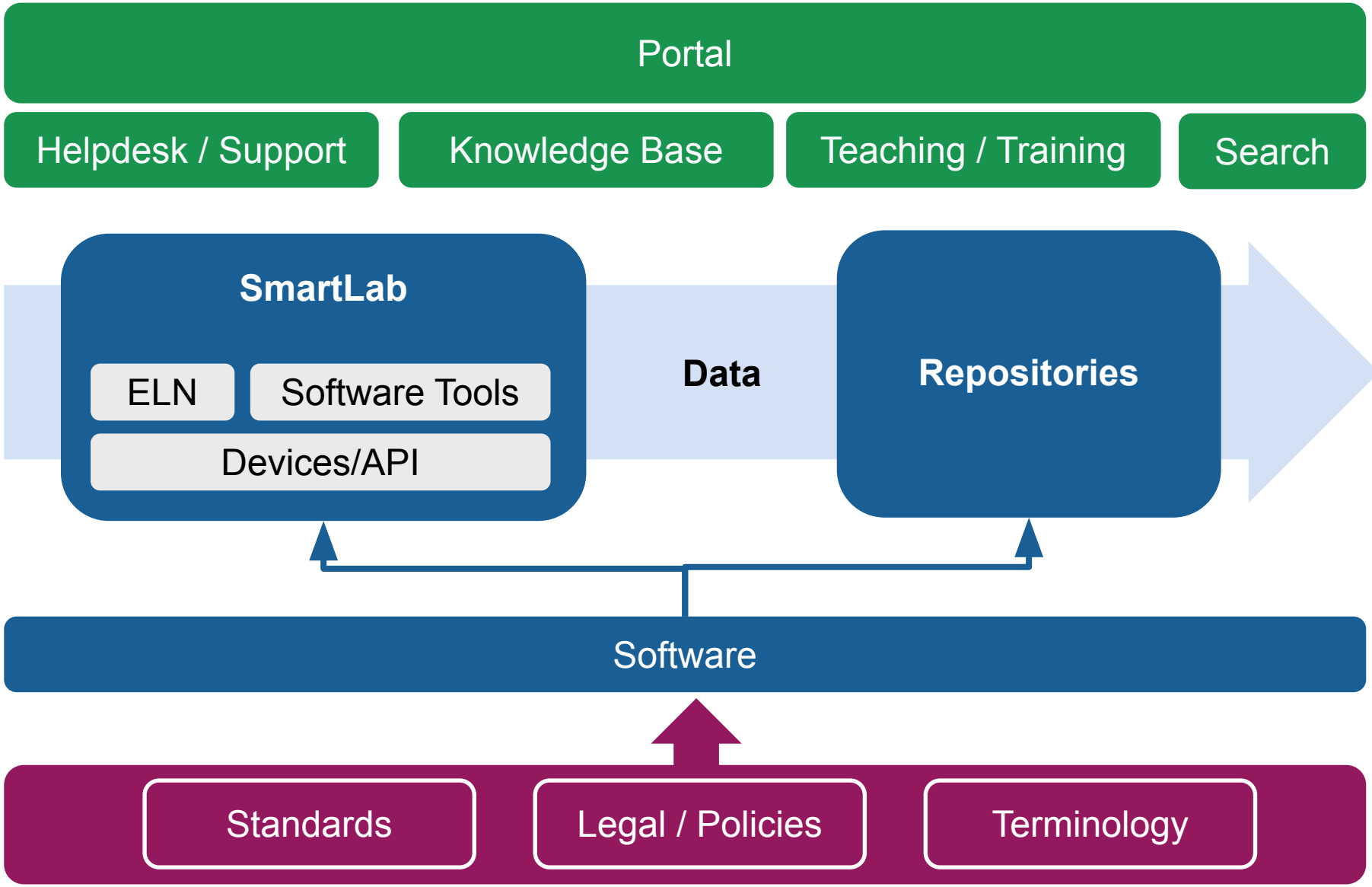
Process & Analytics

Spectroscopy

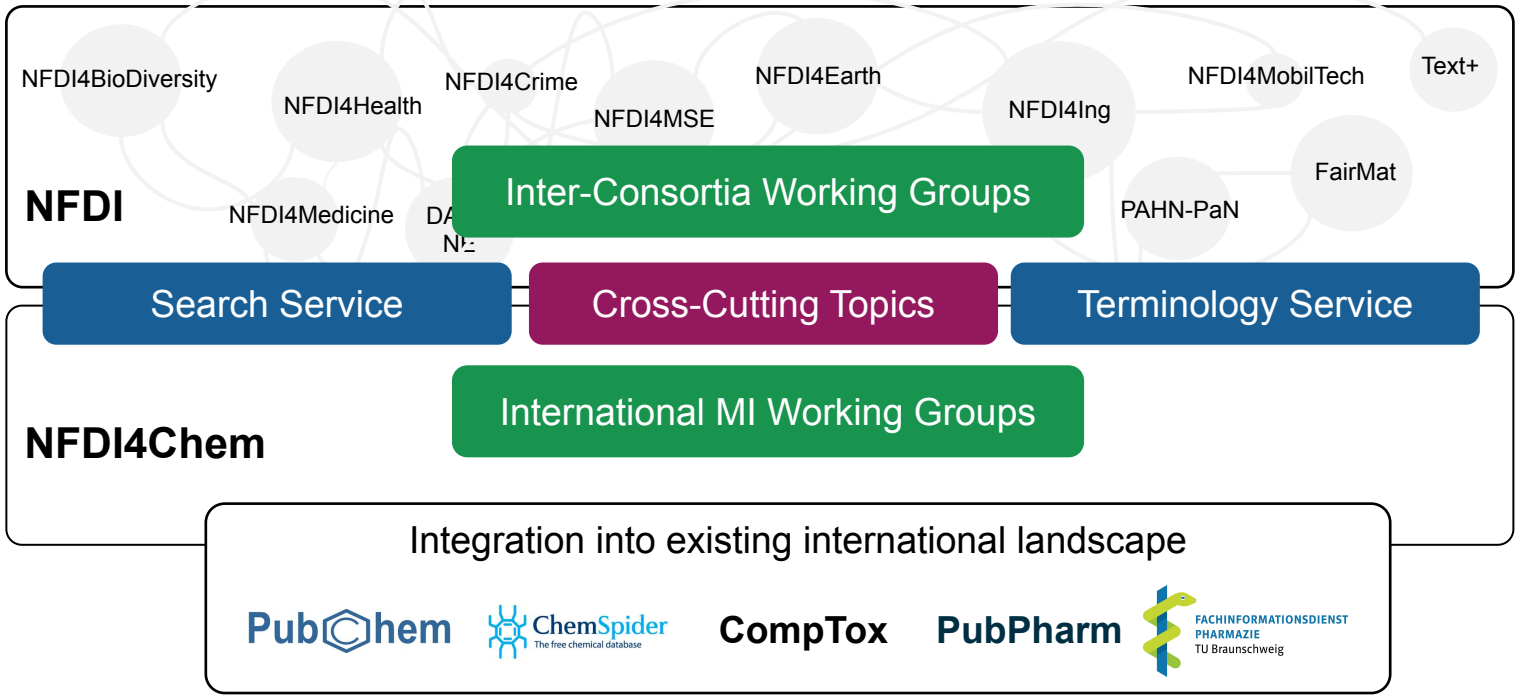
Subdomain-specific

Multi-disciplinary / Generic

Strategy & Resulting Services

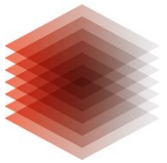


The Role of TIB in NFDI4Chem - Synergies & Cross Cutting Topics



- Infrastructure partner with longterm, sustainable service portfolio
- Expertise in: semantic annotation and linking of research data artefacts
  Standardisation of metadata and data
  Ontology development & curation (together with domain experts)

Activities of TIB within NFDI4Chem



TIB

- Ontology Curation & Development
  - Comprehensive survey of existing ontologies for NFDI4Chem and Chemistry
  - NMR-RD Ontology, RXNO Contribution (Realization of an exemplary procedure with 3rd party maintainer)
- NFDI4Chem Terminology Service (online end of June)
  - Release 1.0 with 18 ontologies, cooperation with NFDI4Health OLS Development
- Integration of Terminologies in NFDI4Chem Services
  - Use Case: chemotion ELN fetches RXNO data from Terminology Service
- Cross-Cutting Topics
  - Co-authoring Declarations on Cross-Cutting Topics, Report on NFDI Cross-Cutting Workshop
  - Shaping the Sektion (Meta)Data, Terminologies and Provenance in NFDI e.V. / NFDI-AAI cross-consortia working group
  - Developing Minimum Information Standards for Chemistry (together with RDA, IUPAC)
- NFDI4Chem Helpdesk Service (in place since April)

NFDI4Chem - Become a member of the Community

Looking for more information on NFDI4Chem?

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