US EU Roadmap
- Nanoinformatics-

Concept and Outline

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Current situation

Europe:

- nanosafety data from more than 60 European and many national projects are stored ad hoc and dispersed over Europe

Nanosafety data are heterogeneous and include:

- Physico/chemical characteristics of NMs
- Toxicity/ Ecotoxicity
- Exposure
- Fate

....

These data could be used

- to perform risk assessment (human and environmental safety)
- for model development
- for grouping
- for safe design and safe innovation
- ...

Objectives for a nanoinformatics roadmap

Objective 1: vehicle for community interaction, to support different stakeholders

Why?
- high amount of money has been spent on nanoEHS so far, future resources are limited
- many different stakeholders (industries, academia, agencies etc.), each with its own objectives & needs

The nanoEHS community needs

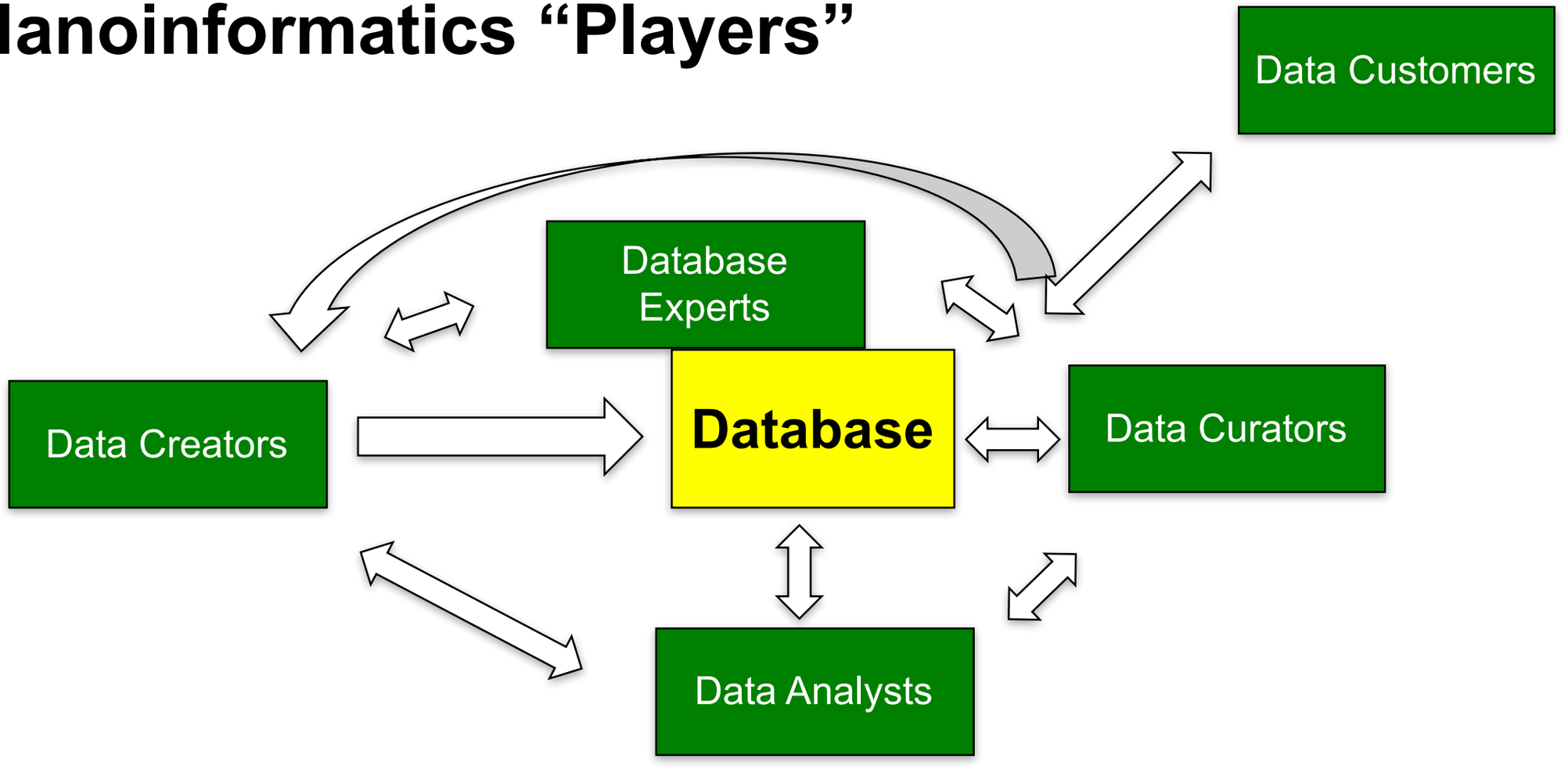
1) to make highest possible use of the currently existing data
2) guidance on which type of research/ which type of data is needed in future
3) a medium to help the community to "self-assemble" & to get to know the different players, their tools as well as their individual needs/ objectives

The nanoinformatics roadmap will support the community to

1) get to know the different stakeholders with their objectives & helps to create a benefit for each
2) describe the nanoinformatics processes and tools
3) give an overview which tools are available to whom & how to use them

Nanoinformatics tools are not only useful for specialized experts, but for all stakeholders!

Nanoinformatics “Players”



...maybe not complete...

Objectives for a nanoinformatics roadmap

Objective 2: **capture, preserve, disseminate all publicly-available NM data (experimental and computational)**

Why:
- avoids remeasurement
- provides access to previous measurements
- assures consistency in reporting of results
- facilitates planning new measurements
- keeps results secure
- increases the ROI for measurement support

Thus, the goal is
- to build and to link different repositories
- to ensure that all publicly-funded NM (measurement) results are deposited

The roadmap will
- raise public awareness of the benefits
- describe how to achieve this goal step- by- step
- explain what kind of infrastructure is needed for this

Objectives for a nanoinformatics roadmap

Objective 3: **Take advantage of existing NM measurement results**

Why:
- To advance nanotechnology and expedite its commercialization
- To help different stakeholders to reach their specific objectives

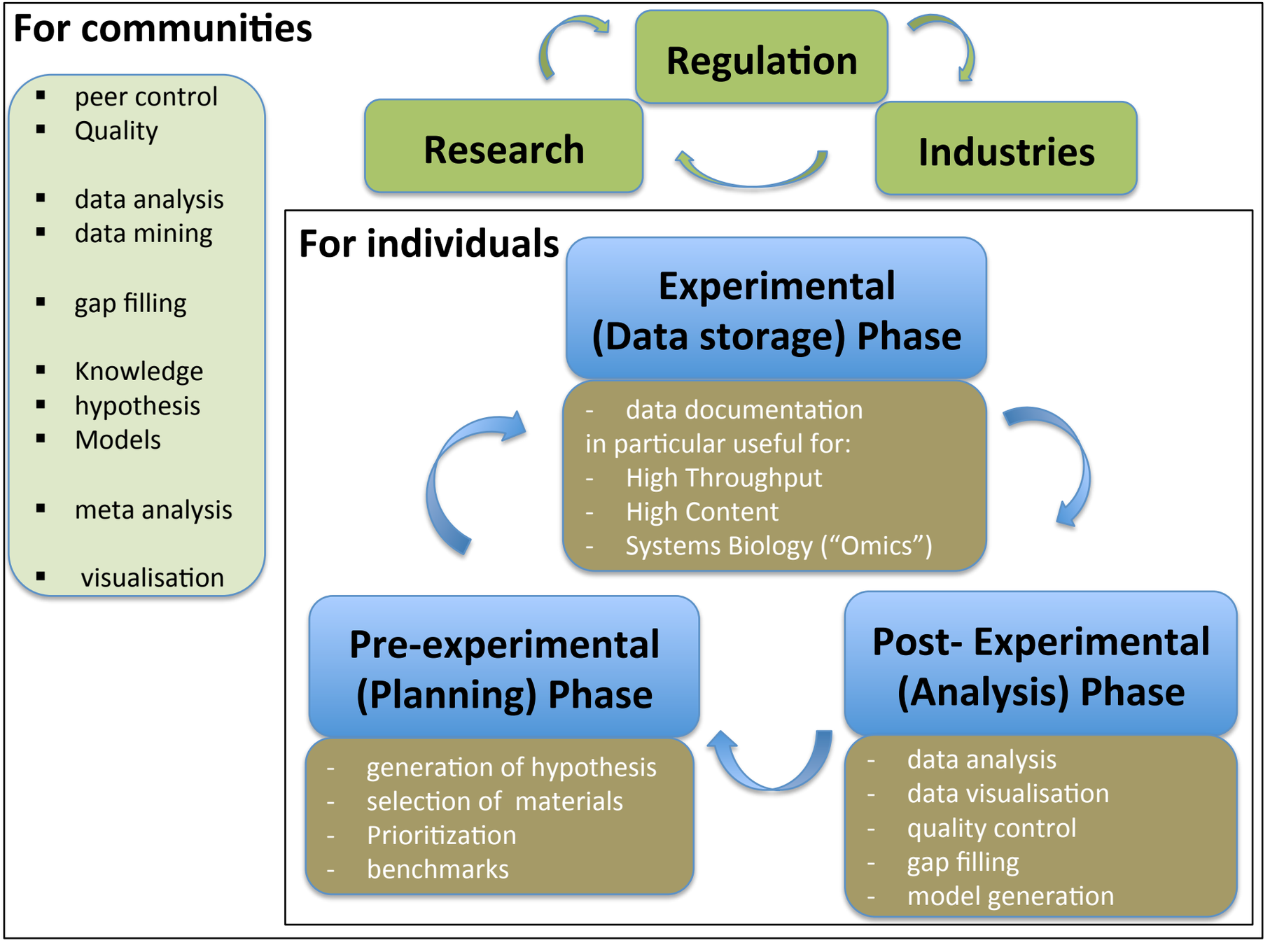
What:
- Develop understanding of results
- Support model development
- Predict properties and performance of nanomaterials
- Correlate results with nanomaterial characteristics
- Correlate results with other functionality
- Advance development of new nanomaterials
- Support Safe-by-Design
- Support decision making
- Support regulation

....

This objective is tightly linked to objective 2.

Objective 4: **Identify specific pilot projects to reach the first three objectives. Describe the way forward (= roadmap)**

Nanoinformatics Processes and Impact



Update until Rheinfelden Meeting

1) Interest in Nanoinformatics 2020 Roadmap expressed by Europe, June 2016 at US-EU COR Meeting (Andrea Haase)

2) U.S. and Canadian participation encouraged

3) Outline discussed over summer

4) First ideas for some chapters circulated in September

5) Intense discussion at 2-Day workshop in Rheinfelden 24 & 25 Oct.

Group Responses at Rheinfelden Meeting

1) Suggested a map of particle history for orienting the discussion

2) discussed issues of nanoform (nanoscale form in U.S.) and visualizing coatings

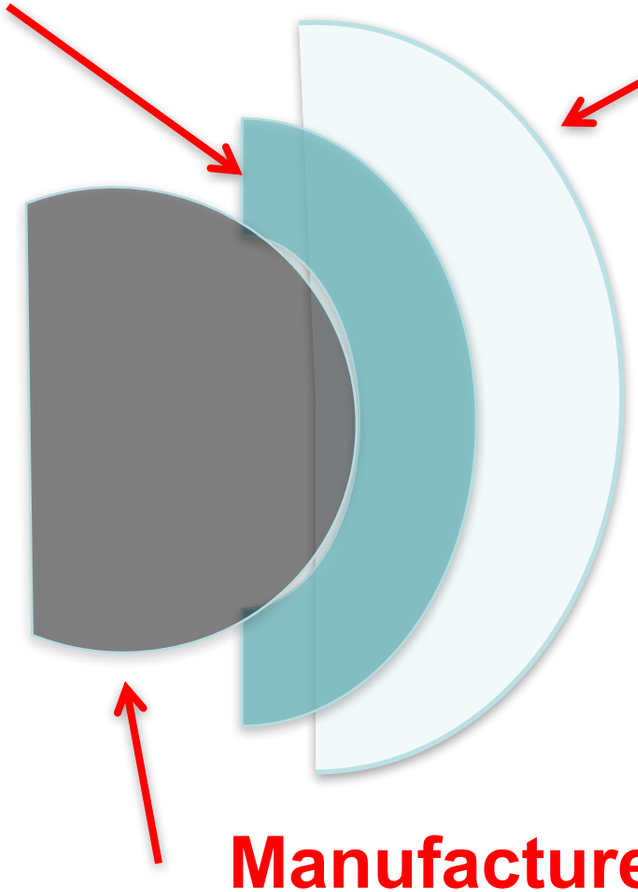
3) proposed and discussed 4 pilot projects

4) did not (yet) address decision tools or bioinformatics

Particle Surface Regions

Nanocoating
Nanolayer

Adsorbed



Layer from Formulation

biologically relevant test medium (proteins like BSA , salts like PO4)

Manufacturer → Formulator → Env. + EHS

Particle/Core/Substance

Comment

Chemical Grouping will become fit-for-purpose , e.g. silica-coated ZnO by

- Traditional chemistry (metal oxide)
- Environmental dispersal (SiO_2)
- Protein Corona formation (SiO_2)
- Toxicity mechanism remains Zn^{+2}

Silica-coating likely stifles sulfidation

Do not know extent of multiple 'groupings'

Particle “Journey”

Nanoparticle

Properties

Formulation
Interactions

Manufacturer
Formulator

Product Life Cycle
Until Release + Environment

Fate/ Exposure
(Modelling)

EHS Testing

1) Test Media Interaction

2) Receptor Interaction

3) MIE

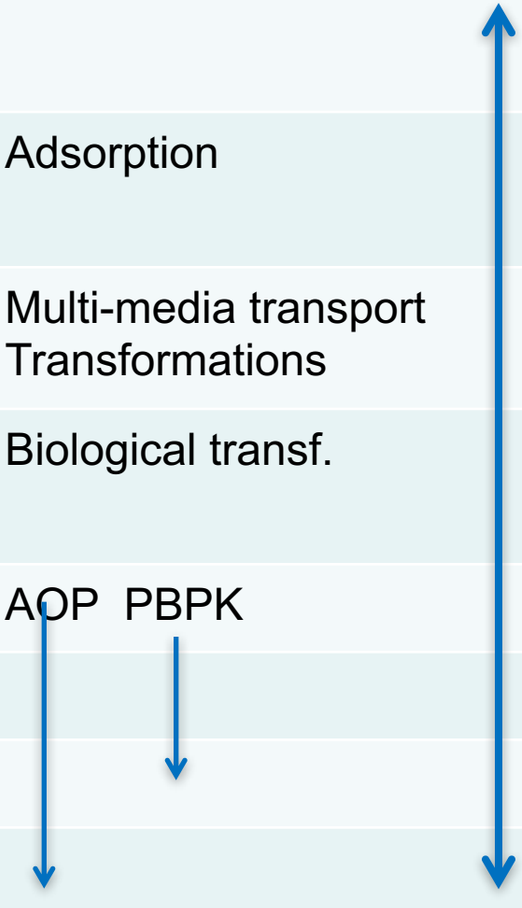
4) Cellular/ Tissue Response

5) Adverse Outcome

6) Population Response

Particle “Journey” & Models & EHS

Models	Stages	EHS
Process & Performance	Particle	Manufacturer/Distributor
Materials Modeling QSAR Cheminfo Modeling ATS	Properties	Performance
Adsorption	Formulation Interactions	Processor/ Formulator
Multi-media transport Transformations	Fate/Exposure	Inhalation/ Oral/ Dermal Air/ Water/ Soil
Biological transf.	Test Media Interactions	Protein or Environmental Corona
AOP PBPK	Receptor	Uptake/ Biodistribution
	MIE	In organism/ Cell
	Response	Cellular/ Tissue Mechanisms
	(Adverse) Outcome	Whole animal
	Population	



Pilot Projects

1) Overview on current or future available databases & access conditions
   - caNano, CEIN, CEINT "now"; NANoREG completion + six months; leading to vision for Open Science

2) Dissolution
   - Proposed as decision tool; determine industry interest; clarify regulator requirements; consider ageing; serve as coordinator

3) Training
   - Survey current actors; incorporate help desk and P.I. proposals from NanoCommons and U.S.

4) Infrastructure(s)
   - Instances of characterization and Ontology efforts at ASTM
   - Revisting ISA-TAB-nano and NANoREG & JRC Templates (extend to other datasets focusing on error expressions, metadata parameters, etc.)
   - Incorporate UDS considerations
   - Address AOP and chemical grouping

Short Outline

Section 1: Data Gathering and Data storage

a) Quality of Data
b) Data curation
c) Databases: ontologies, requirements, standards
d) metadata
e) Challenges: e.g. missing standards, heterogeneous datasets

Section 2: Data Analysis

a) **Material modelling**
- Modelling physical/ chemical descriptors of NM
- Explore how NM descriptors depend on the underlying physics and chemistry

b) **Chemoinformatics**
- Similarity Analysis
- Gap Filling (e.g. Read Across, QSAR)
- For exposure assessment & exposure modelling
- PBPK

c) **Bioinformatics** & AOP‘s

d) **Guidance** for other communities
- for pre-experimental planning, data storage, data analysis etc.
- challenges
- explain possible benefits and applications for different stakeholders (e.g. academia, regulatory agencies, industry)

Section 3: Data Accessibility & Data Exchange

Standards for information exchange

Section 4: Current Network

Overview on most important projects ongoing projects in EU and US

Training possibilities

Workshop and conference series

Section 5: Roadmap

Short term projects or action points

Medium term projects

Long Term projects (up to 2030)

Links

The European Materials Modelling Council

EMMC Roadmap 2016

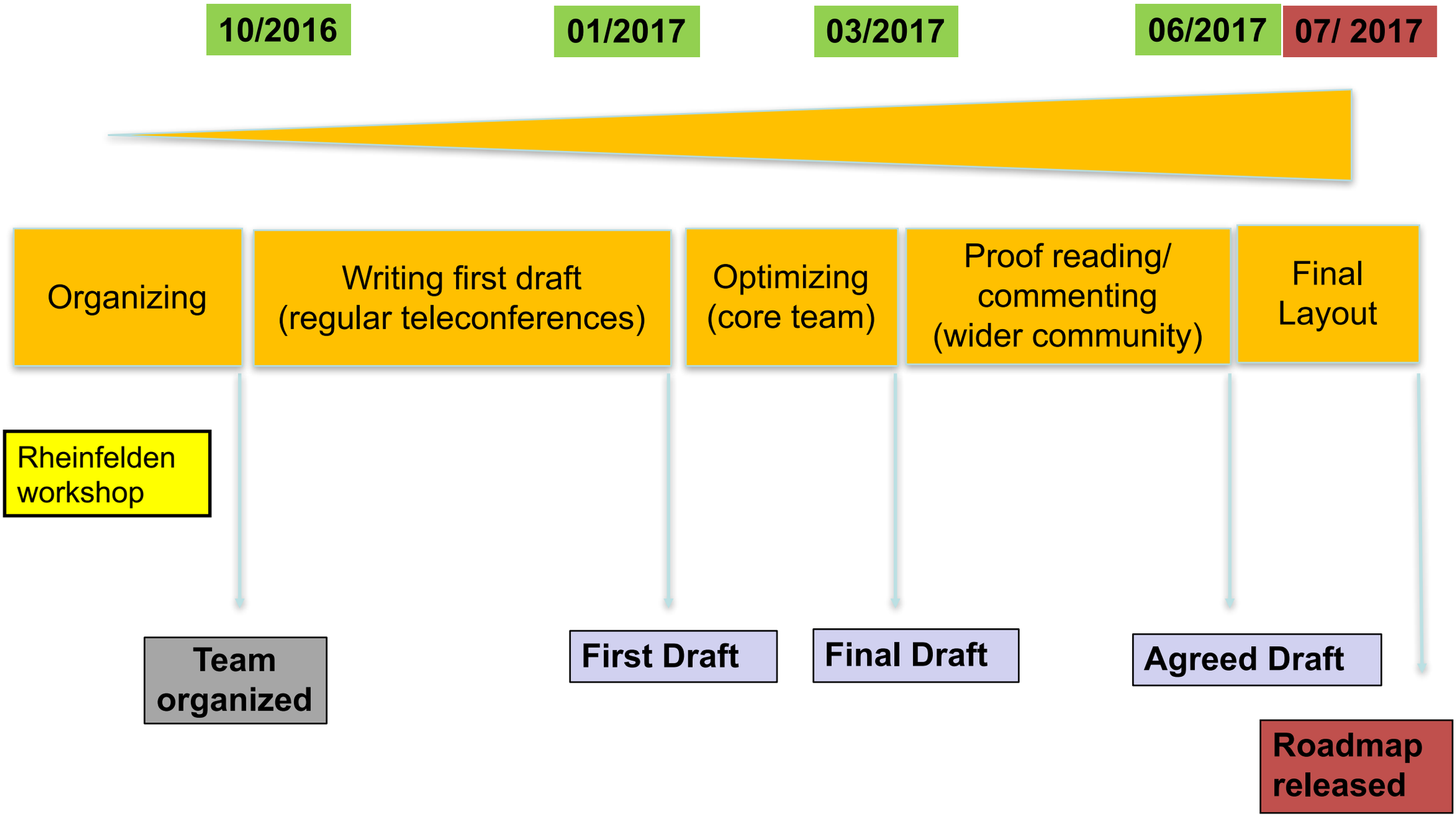
The EMMC seeks to update its RoadMap for Materials Modelling to propose new topics aimed at recommendations for the 2018-2020 NMBP Programme.

As a first step the EMMC started an open survey to collect views on what materials modelling developments are required in order to respond to the application needs of the European industry. The inputs collected via this survey will lay the groundwork for elaboration of the EMMC RoadMap 2018-2020, a process which will start during a meeting in Brussels on 20th May 2016, with participation (by invitation) of many active survey contributors.

EMMC

*The **European materials modelling council (EMMC)** is a community driven bottom-up action to connect all existing material modelling activities and stakeholders in Europe*. The EMMC aims to network with all existing materials modelling related activities in Europe and make use of the EMMC network to complement these activities

Timeline


10/2016
01/2017
03/2017
06/2017
07/ 2017
Organizing
Writing first draft (regular teleconferences)
Optimizing (core team)
Proof reading/ commenting (wider community)
Final Layout
Rheinfelden workshop
Team organized
First Draft
Final Draft
Agreed Draft
Roadmap released

Core Team (to be extended)

Name		Affiliation
Andrea Haase	EU	**German Federal Institute for Risk Assessment (BfR)**
Frederick Klaessig	US	**Pennsylvania Bio Nano Systems**
Sabina Halappanavar	CAN	**Health Canada**
Mark D. Hoover	US	**US NIOSH**
Tomasz Puzyn	EU	**University of Gdansk**
John Rumble	US	**P+R Data Service**
Pietro Asinari	EU	**Politecnico di Torino & European Materials Modelling Council**
Claus Svedson, David Spurgeon, Marianne Matzke	EU	**NERC-CEH**
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Christine Hendren	US	**Duke CEINT**
Nina Jeliazkova	EU	**IDEA**
Barry Hardy, Lucian Farcal	EU	**Douglas Connect**
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Extended Team (not complete)

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Treye Thomas	US	**US CPSC**
Anil Patri	US	**US FDA**
Stacey Stanridge	US	**US NNCC**
Teresa Fernandes	EU	**Herriot Watts University of Edingburgh**
Bengt Fadeel	EU	**Karolinska Institute**
Hubert Rauscher, Hugues Crutzen	EC	**JRC**
Robert Rallo	US	

Thank you very much!

Please feel free to join us.
We are looking for volunteers.