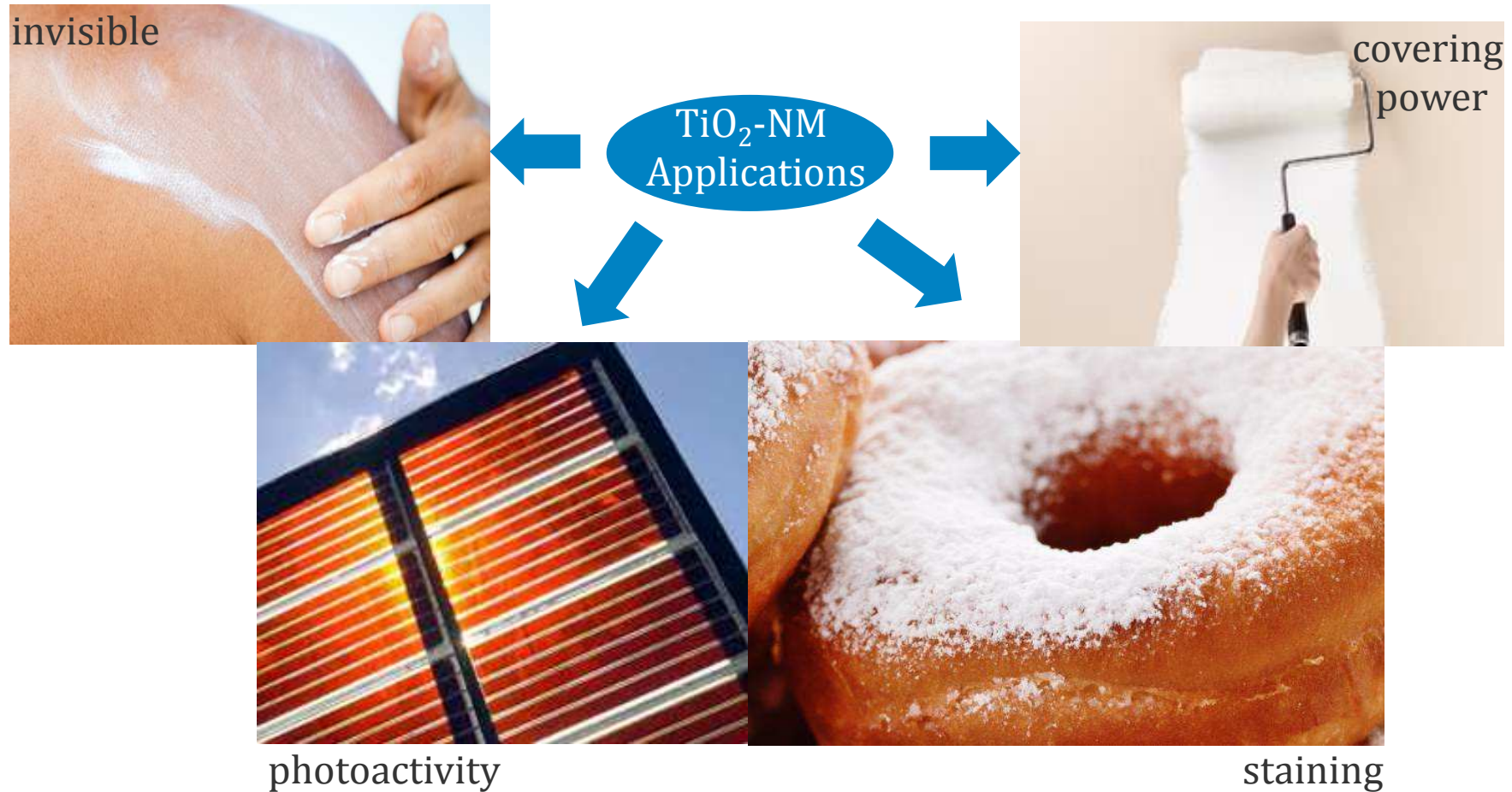


▶ SAFE BY DESIGN FOR INNOVATIVE NANOMATERIALS

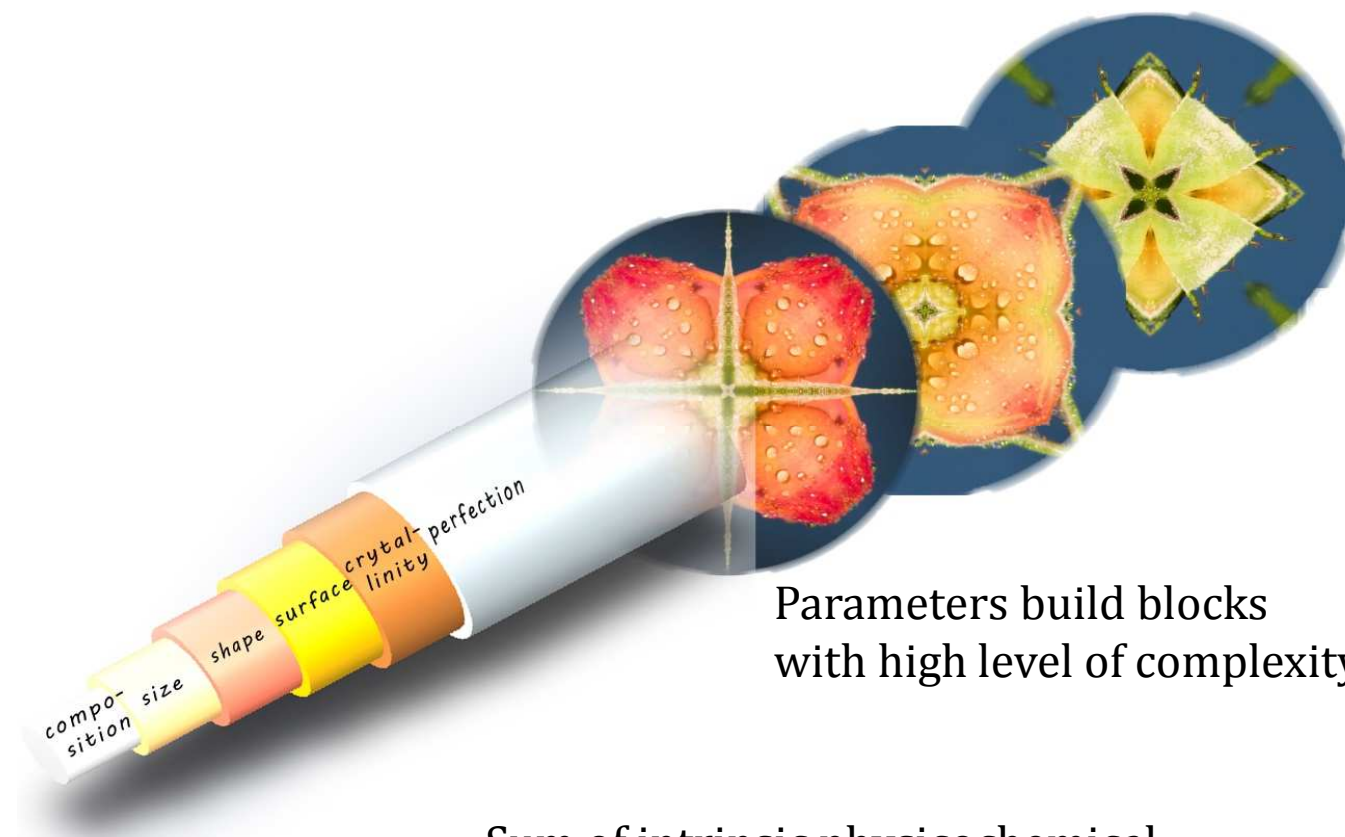
Isabella Tavernaro, Petra Herbeck-Engel, and Annette Kraegelo
NanoSafe 2018, Grenoble, 7th November 2018

► MOTIVATION

one composition: several properties \Rightarrow different applications



▶ IDENTITY OF NANOMATERIALS



Parameters build blocks
with high level of complexity

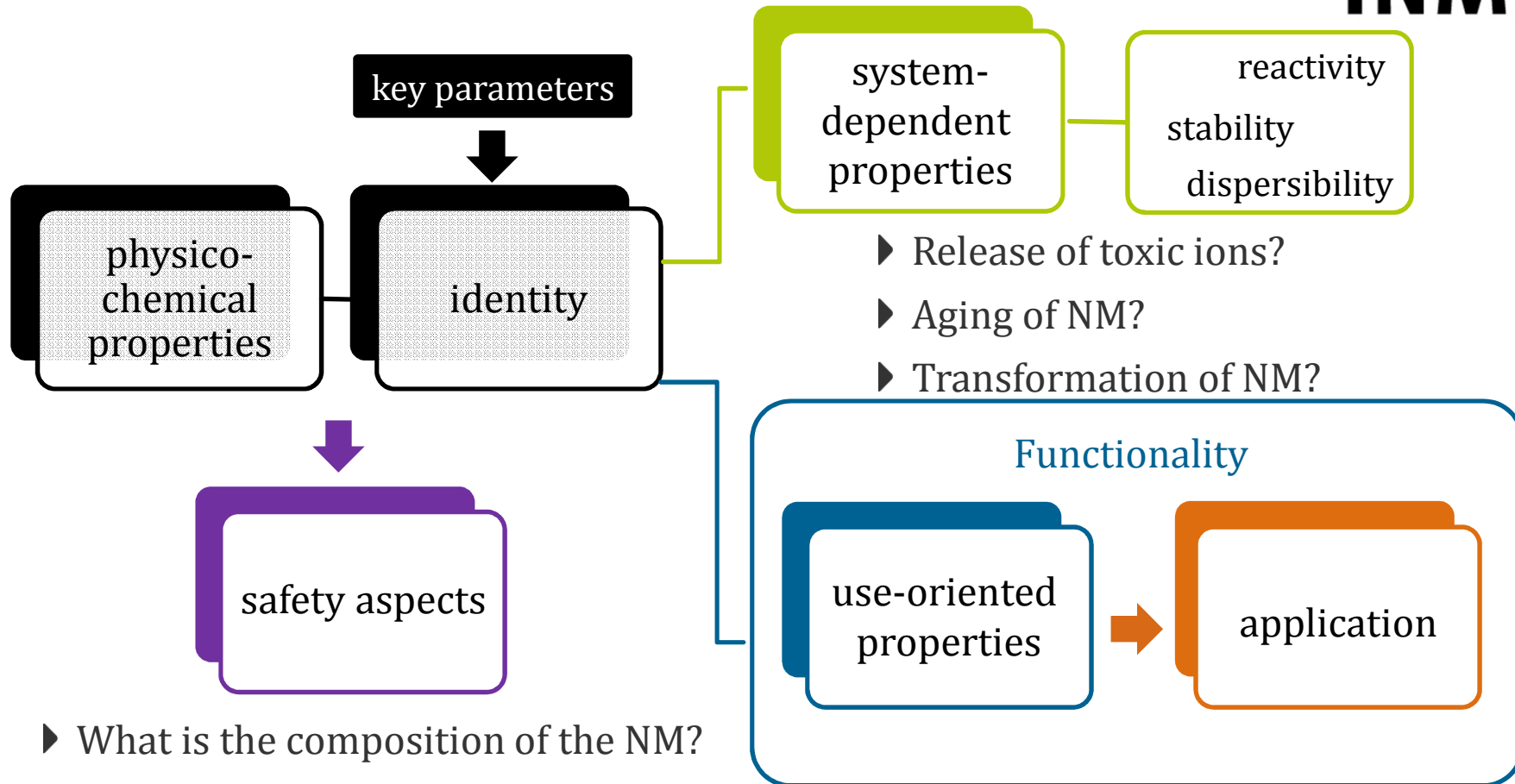
Sum of intrinsic physicochemical
parameters

⇒ databases and grouping approaches

| |
|----------------------|
| composition |
| elements |
| doping |
| density |
| size |
| dispersity |
| aspect ratio |
| shape |
| dimensionality |
| spherical |
| porosity |
| crystallinity |
| amorphous |
| surface |
| charge |
| surface area |
| surface allocation |
| roughness |
| perfection |
| impurities |

Ozin, G. A., Nanomaterials Kaleidoscope – Building a Nano-chemistry Periodic Table. *Nanochemistry Views* **2013**, 114-123.

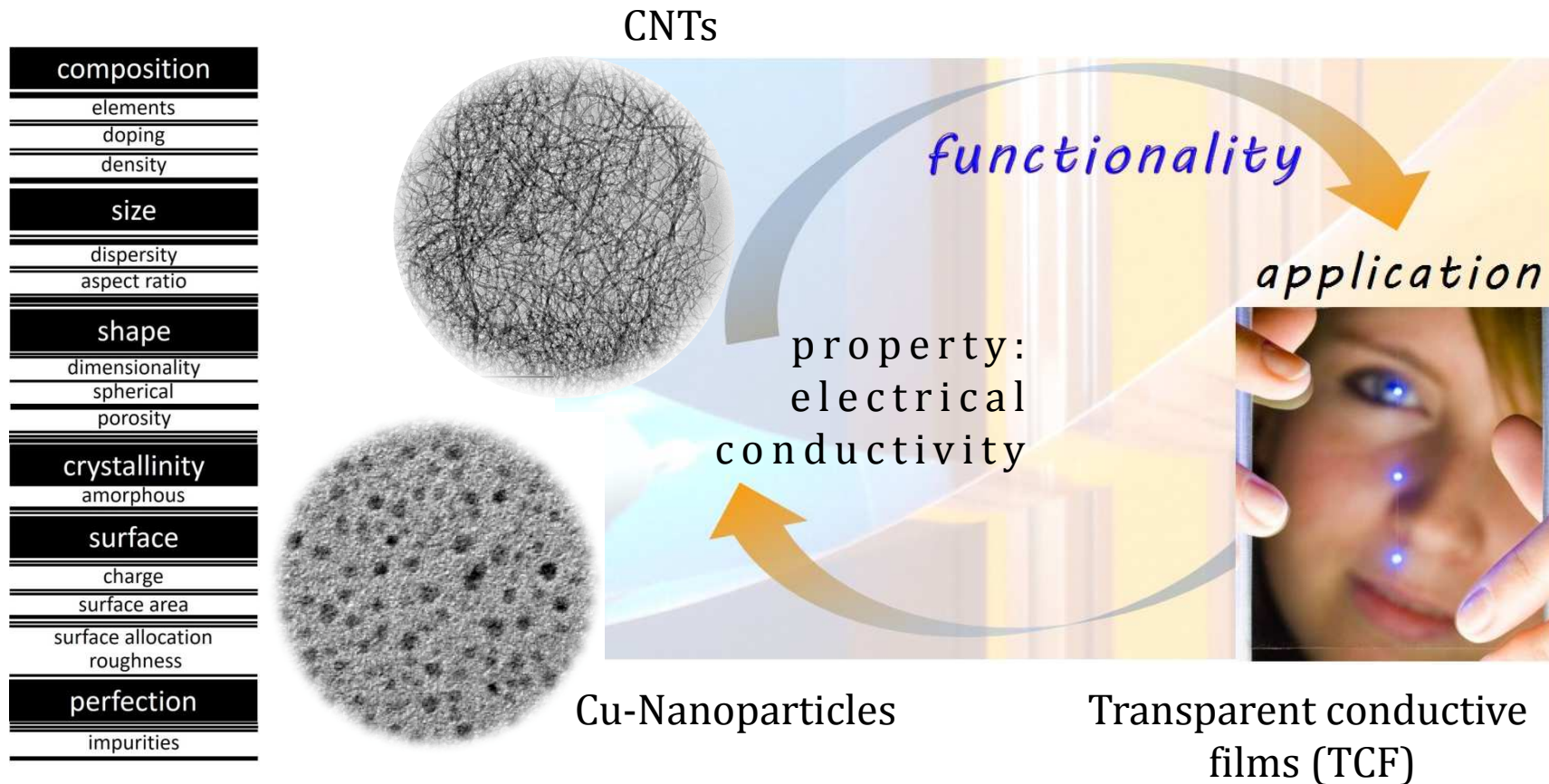
▶ IDENTITY & RELATED PROPERTIES



- ▶ What is the composition of the NM?
- ▶ What is the size of the NM?
- ▶ What is the shape of the NM?

▶ FUNCTIONALITY

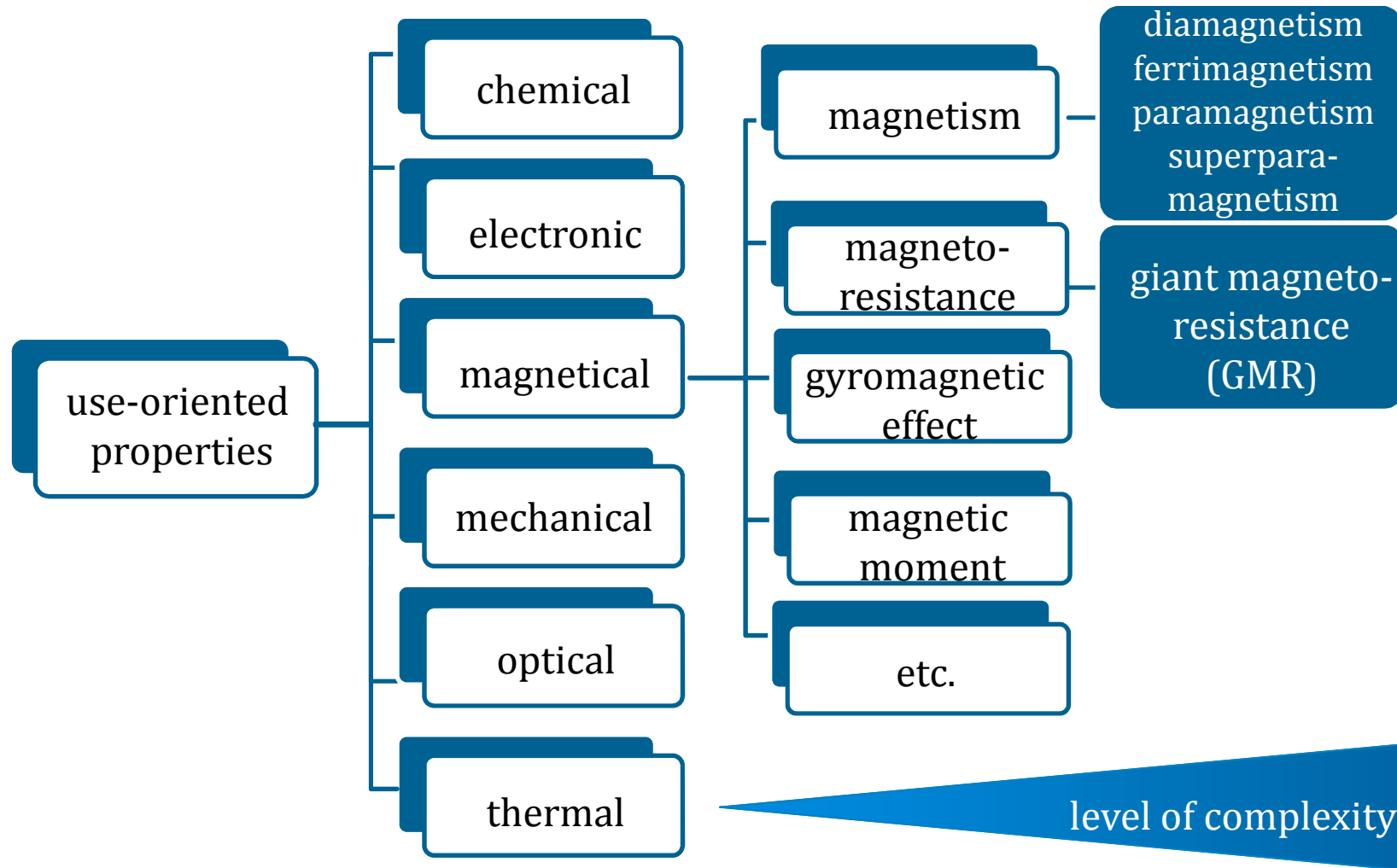
Definition



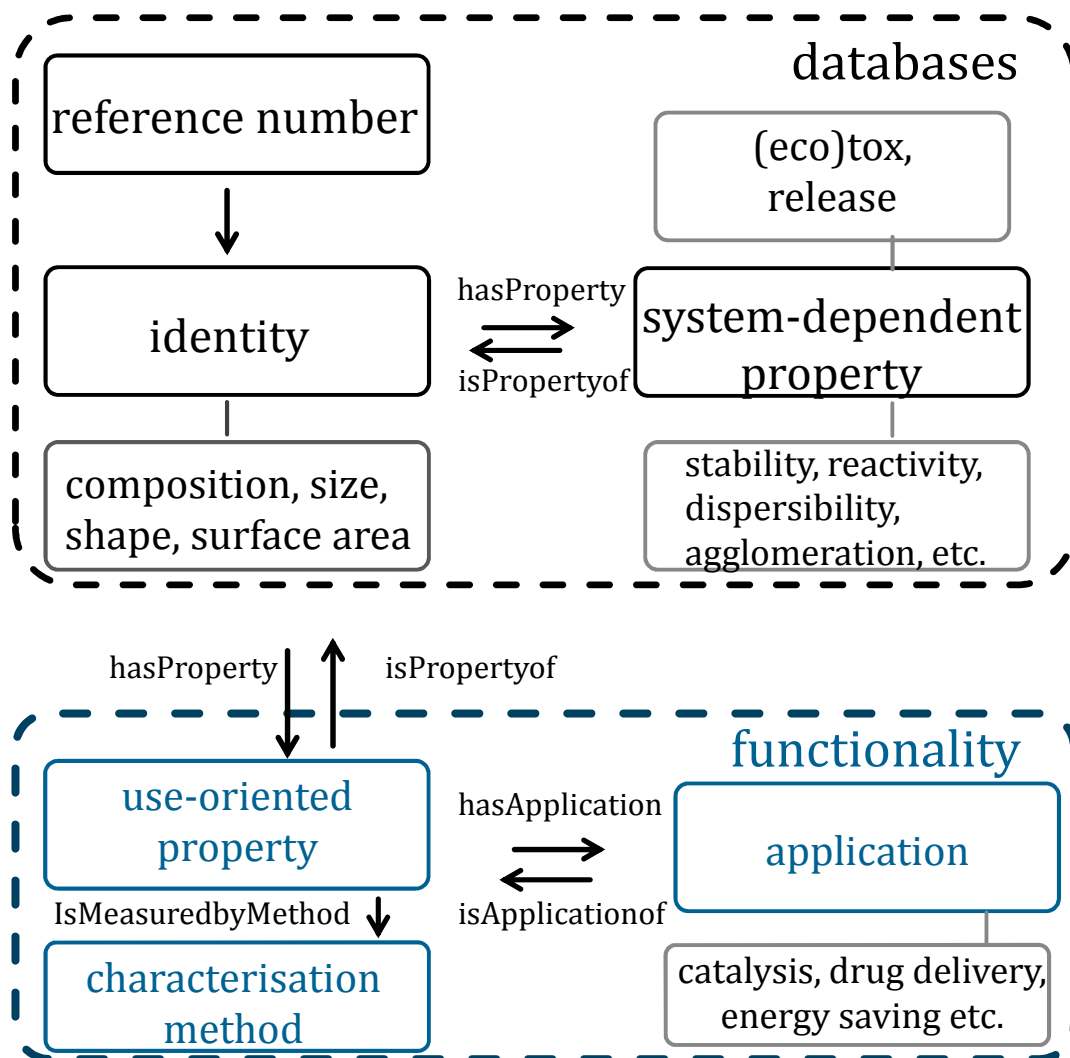
Functionality (quality of being useful)

defines the relationship between use-oriented properties and application

▶ SYSTEMATIC INVENTORY OF USE-ORIENTED PROPERTIES



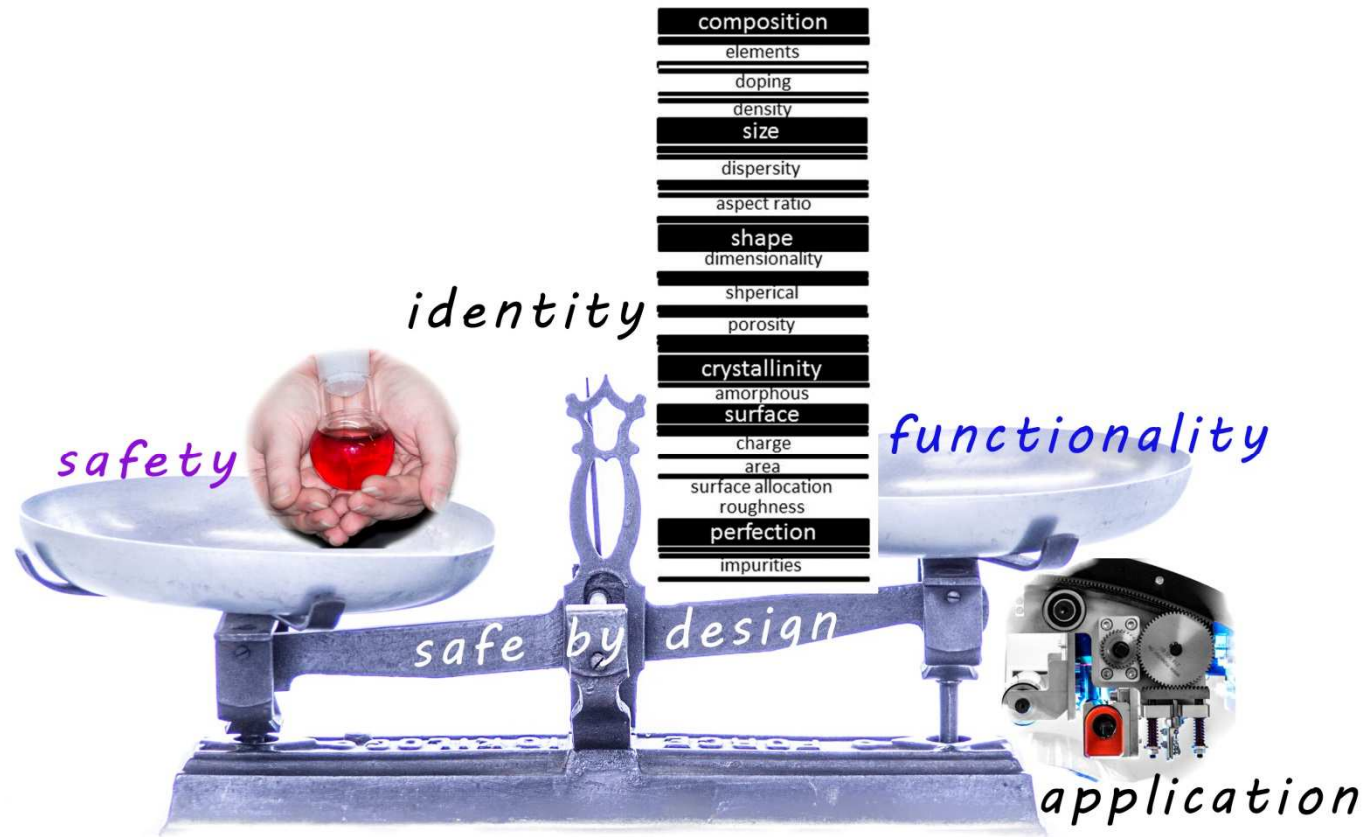
▶ IMPLEMENTATION INTO DATABASES



| Endpoints | Endorem® |
|--------------------------------|---|
| functionality | |
| magnetical properties | yes |
| magnetism | yes (paramagnetism) |
| magnetic relaxation | Yes relaxivity [L/mmol-s]: r1=40.0 r2=160 applied magnetic field [T]: B ₀ =0.47 |
| resulting field of application | superparamagnetic contrast agent for magnetic resonance imaging; contrast effect T2 |

▶ SAFE BY DESIGN

Interaction of identity, functionality and safety

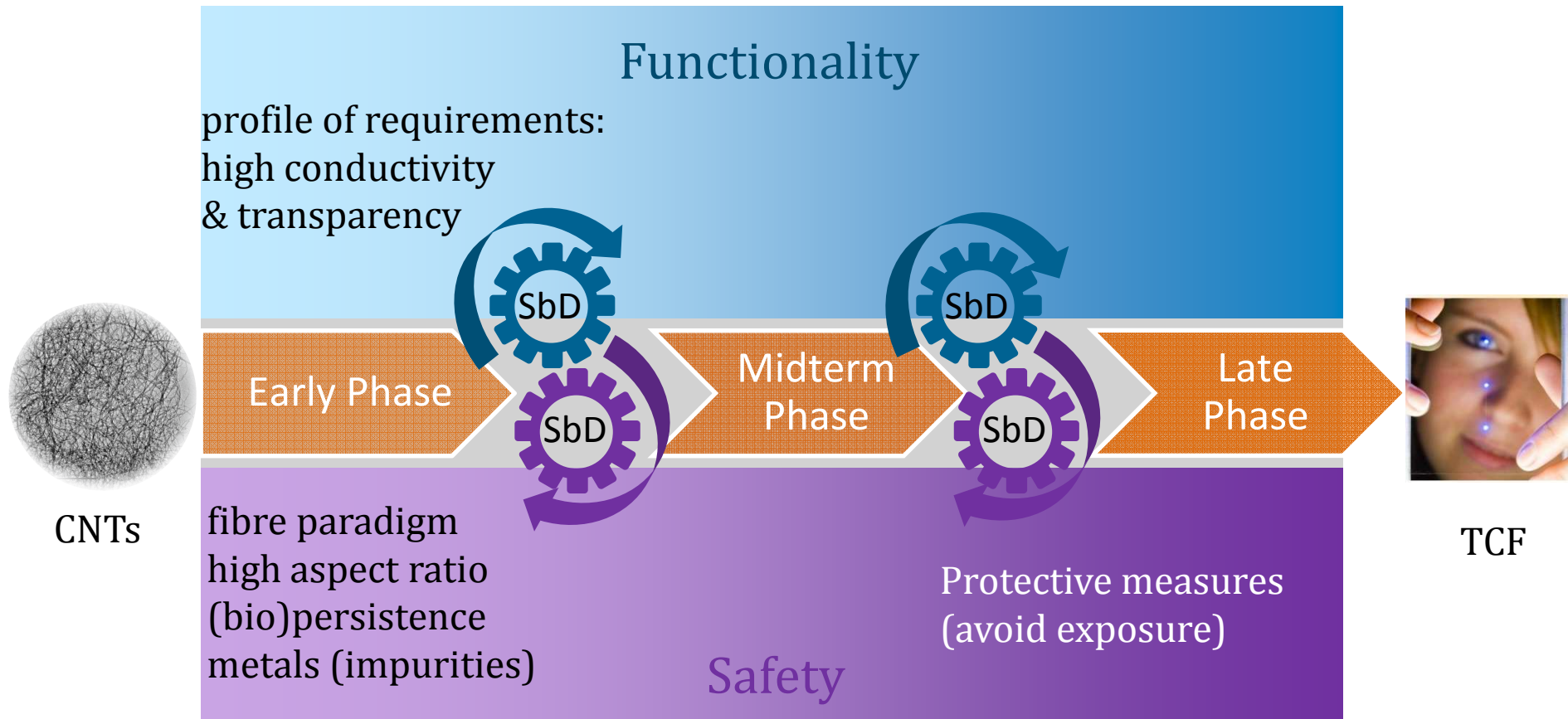


How does the tuning of a particular property influences safety and functionality?

► IMPLEMENTATION OF SAFE BY DESIGN

Example: transparent conductive films (TCF)

ITO (indium tin oxide): excellent optoelectronic properties
In scarcity, high costs, brittleness



► SBD MEASURES: PROCESSING

analyse and optimise processing

- ✓ reduced T
- ✓ reduced amount of catalyst
- ✓ less byproducts

alternative processing

- ✓ without or fixed catalyst
- ✓ synthesis in liquids



► SBD MEASURES: MATERIAL

safety

functionality

modification of material

- ✓ functionalisation
- ✓ doping

alternative materials

- ✓ graphene
- ✓ metallic nanomaterials
- ✓ polymers (i.e., PEDOT)



▶ TAKE HOME MESSAGE



SbD necessarily needs to address **both functionality and safety aspects** to achieve or exceed functional performance of NMs and their application, while minimising inherent hazard potential and avoiding exposure to human and environment at all stages of the life cycle.

- ▶ Understanding of the complex interaction between safety, identity and functionality
- ▶ Design tailored NMs with an optimal balance between functionality and hazard or exposure
- ▶ Establishment of SbD as an important pillar in the development of NMs

ACKNOWLEDGEMENT

NanoReg²



This work is part of the NanoReg II project and has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement 646221.

Cornelle Noorlander
Blanca Suarez-Merino
Susan Dekkers
Thies Oosterwijk
Nina Jeliaskova
Cesar Merino
Araceli Sanchez
Isabel Rodriguez-Llopis
WP3 Partners

 **THANK YOU FOR YOUR KIND ATTENTION**

► IMPLEMENTATION OF SAFE BY DESIGN

SbD Principles



NR1 analyse and optimise
NR2 determine identity
NR3 design out hazard
NR4 avoid exposure
NR5 take on state of the art
NR6 implement SbD early

Results:

- reduce risks and uncertainties
- modifying the material or process rather than using protective measures
- add-on for existing innovation processes

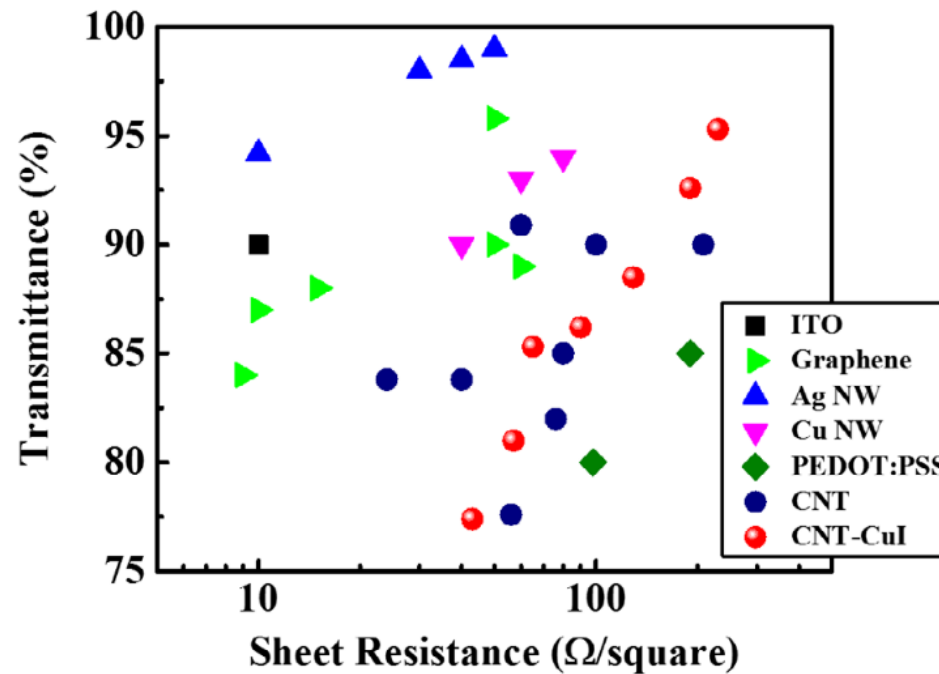


Figure 4. Plot of specular transmittance versus sheet resistance for the best performances of CNT-based TCFs.[96,102,104] Values for commercial ITO, the best TCFs using graphene,[28–31] Ag NW,[19] Cu NW [18] and PEDOT:PSS [12] are provided for comparison.

Y. Zhou and R. Azum, *Sci. Technol. Adv. Mater.*
2016, 17, 493.