

Advanced material properties to support (eco)toxicological safety assessment

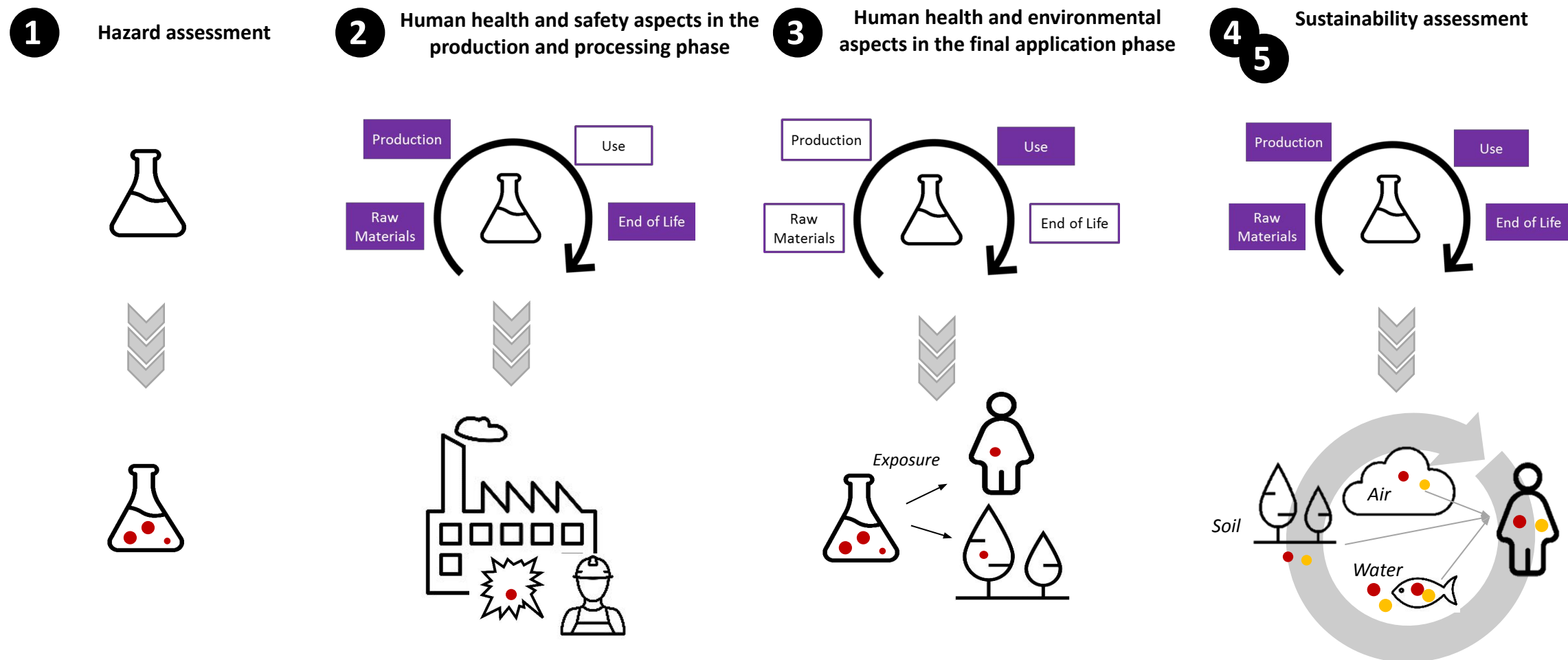


Ca' Foscari
University
of Venice

Prof. Elena Badetti



Safe and Sustainable by Design (SSbD) framework



The concept of Risk



HAZARD “is anything that has the **potential** to cause **harm**”

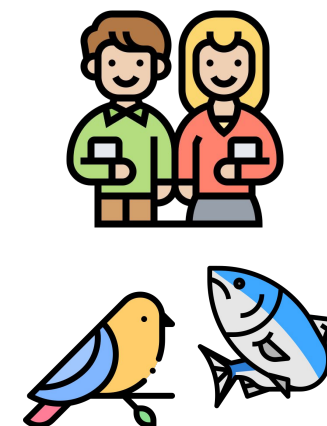
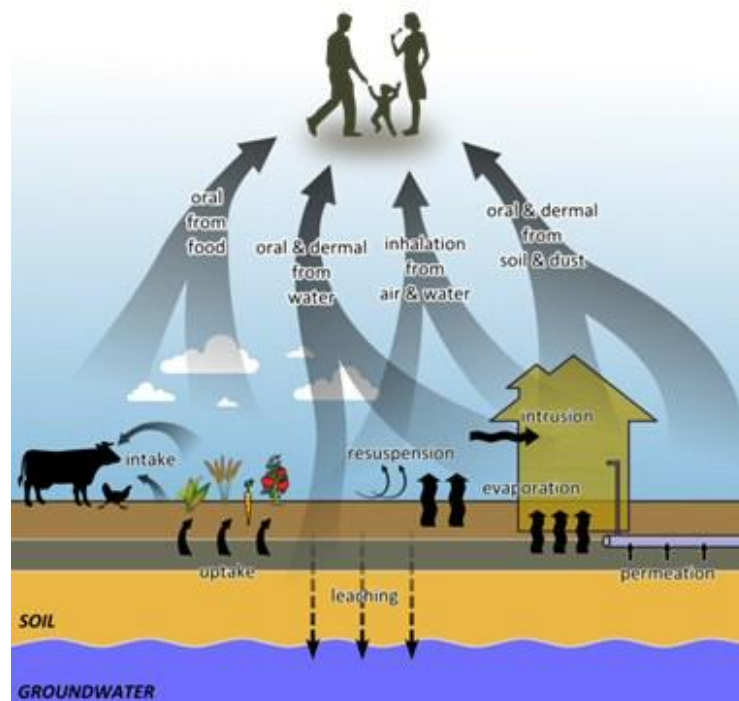
RISK “is the **likelihood** that a hazard will cause **harm**”

$$\text{Risk} = f(\text{Hazard}, \text{Exposure})$$

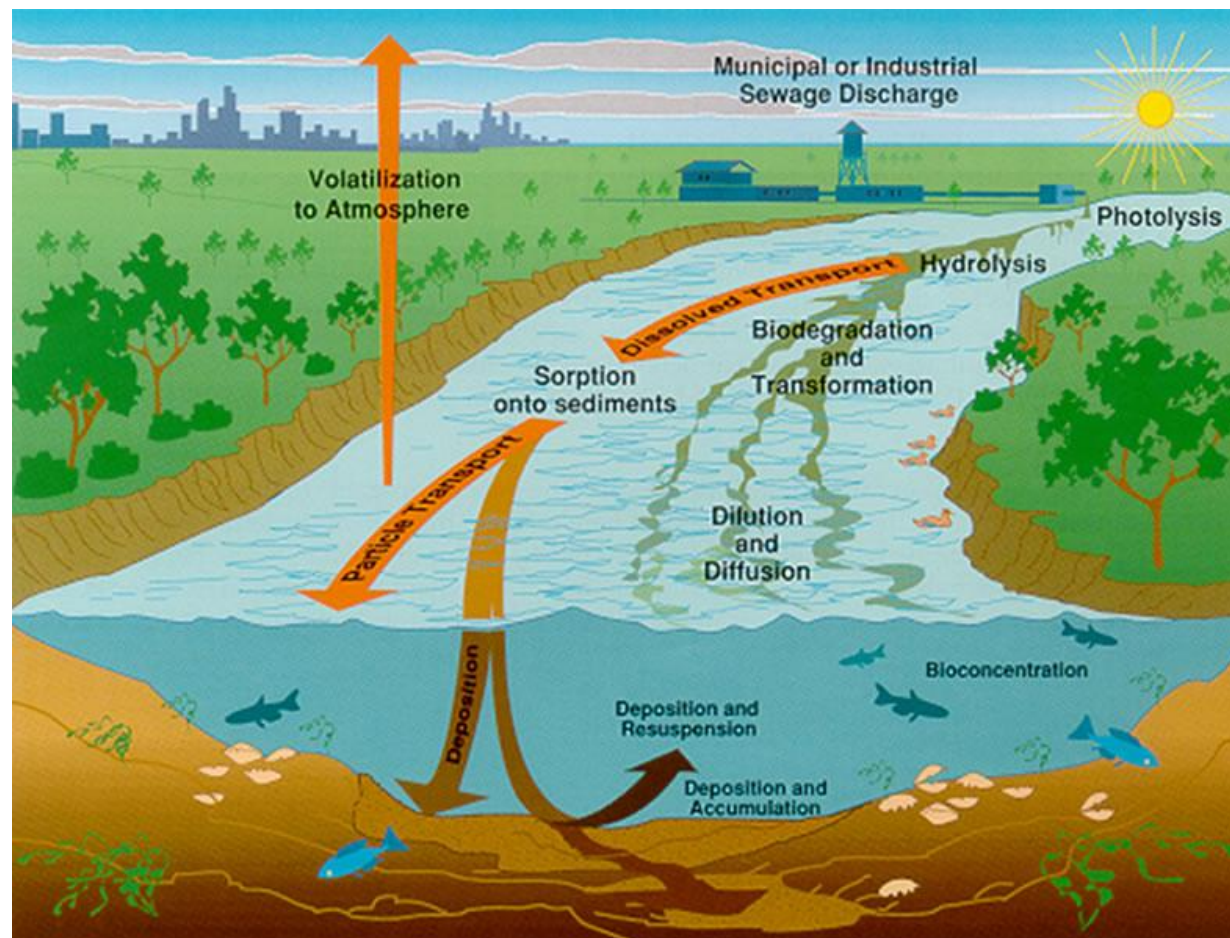
Environmental risk assessment

SOURCES**PATHWAYS****TARGET**

Emissions

Exposure
concentrationHumans
Ecosystems

Physicochemical properties of chemicals influencing (eco)toxicity



Handbook of Environmental Chemistry (2015) vol 46. Springer, Cham. DOI: 10.1007/698_2015_5012

Physicochemical properties of chemicals influencing (eco)toxicity

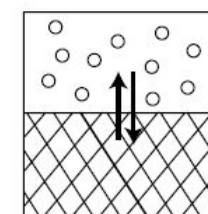


They determine how:

- the substance interacts with the living organism (**toxicokinetics**: absorption, distribution, metabolism, elimination)
- they exerts their harmful effects (**toxicodynamics**)

Physicochemical properties of chemicals influencing (eco)toxicity

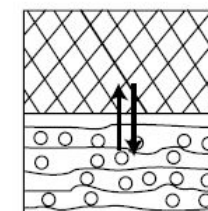
- **Solubility** (in water or in lipids) □ absorption, distribution, bioaccumulation



Gas
↕
Pure liquid
or solid

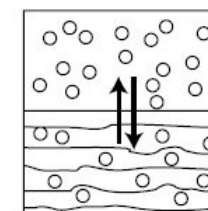
Compound
property

Vapour
pressure



Pure liquid
or solid
(sat. with water)
↕
Saturated aqueous
solution

Aqueous
solubility

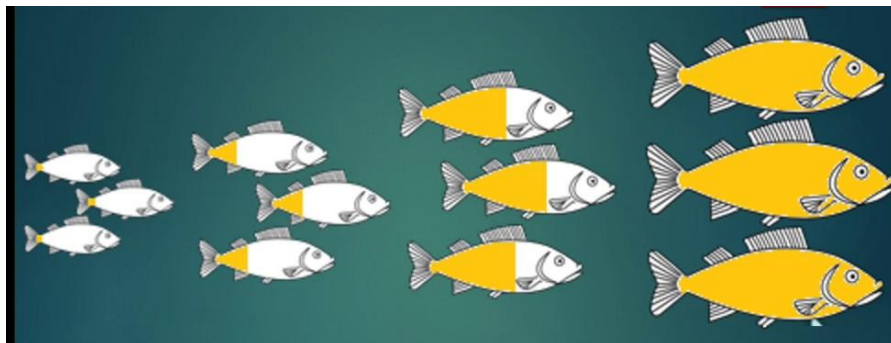
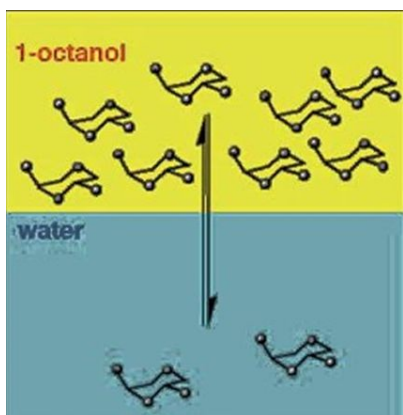


Gas (air)
↕
(Dilute) aqueous
solution

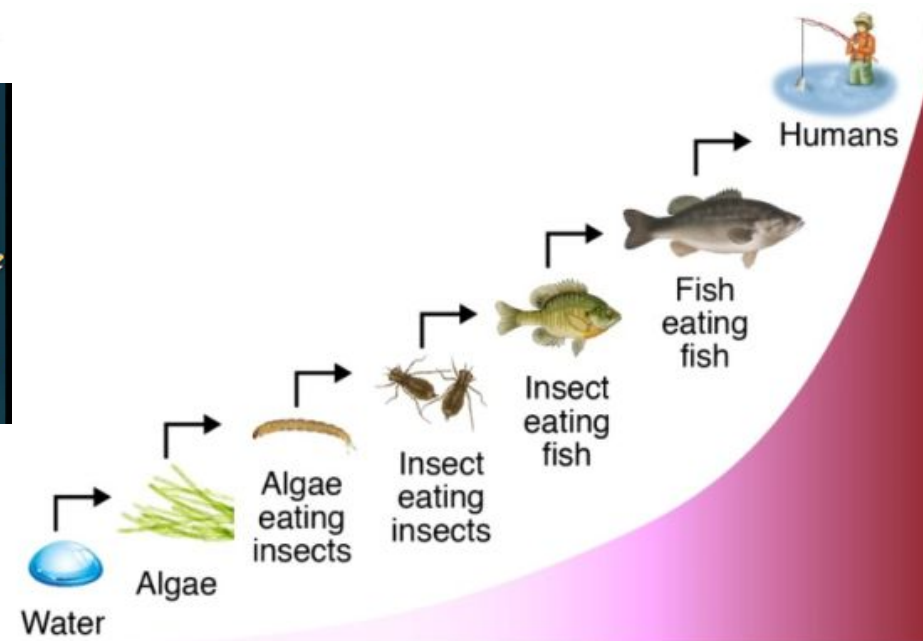
Air-water
partition constant
(Henry constant)
Air-water
distribution ratio

Physicochemical properties of chemicals influencing (eco)toxicity

- **Solubility** (in water or in lipids) □ absorption, distribution, bioaccumulation

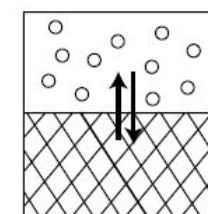


$$K_{OW} = \frac{C_{Octanol}}{C_{water}}$$



Physicochemical properties of chemicals influencing (eco)toxicity

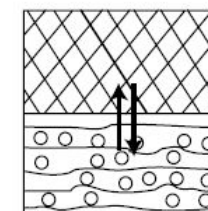
- **Solubility** (in water or in lipids) □ absorption, distribution, bioaccumulation
- **Molecular weight** □ absorption and elimination
- **Degree of ionization/pKa** □ absorption and elimination
- **Volatility/Vapor pressure** □ inhalation toxicity
- **Chemical Reactivity / Stability** □ interaction with biological macromolecules / persistence



Gas
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Pure liquid
or solid

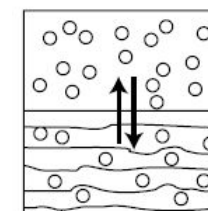
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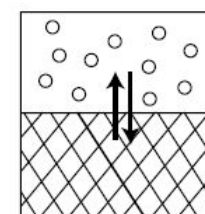


Gas (air)
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(Dilute) aqueous
solution

Air-water
partition constant
(Henry constant)
Air-water
distribution ratio

Physicochemical properties of chemicals influencing (eco)toxicity

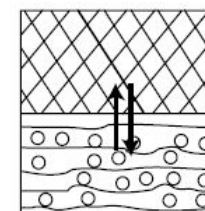
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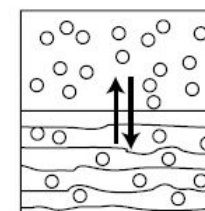
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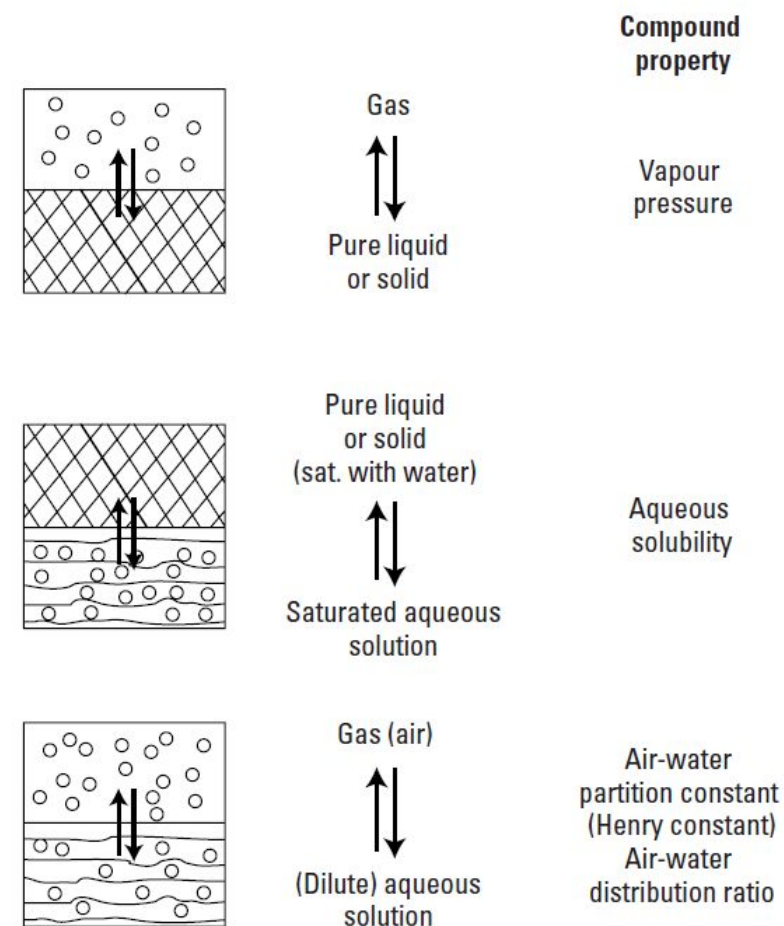


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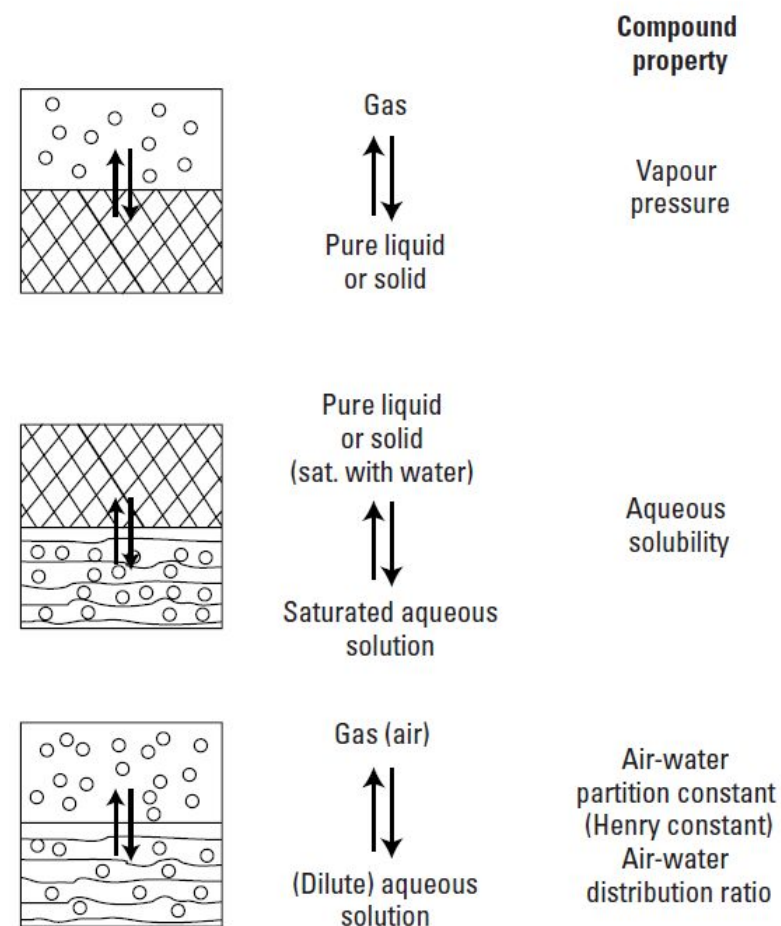
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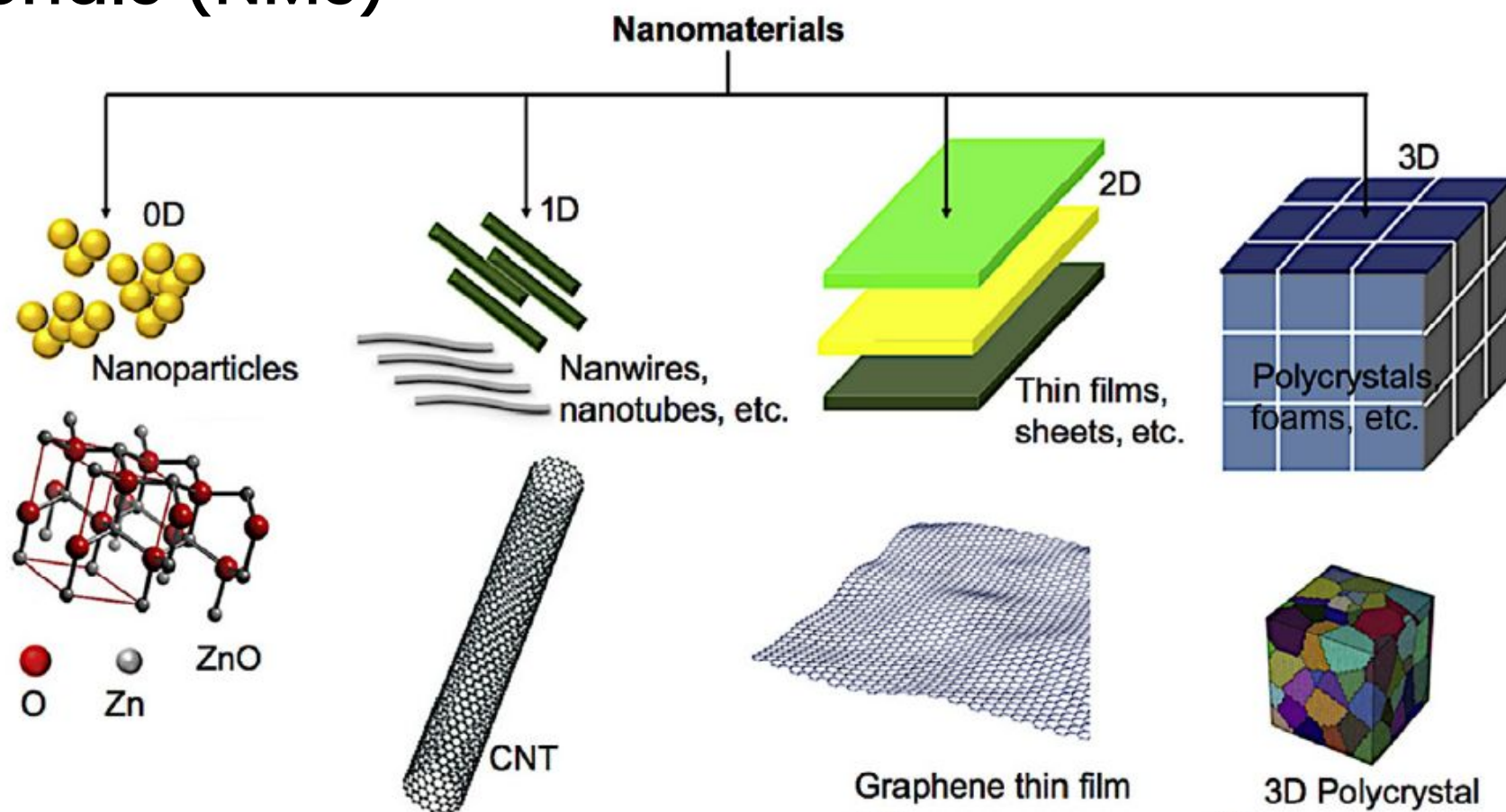


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Nanomaterials (NMs)



Polymer Science and Nanotechnology, Fundamentals and Applications,
Chapter 15 - Nanomaterials properties 2020, Pages 343-359

Physicochemical properties of NMs influencing (eco)toxicity



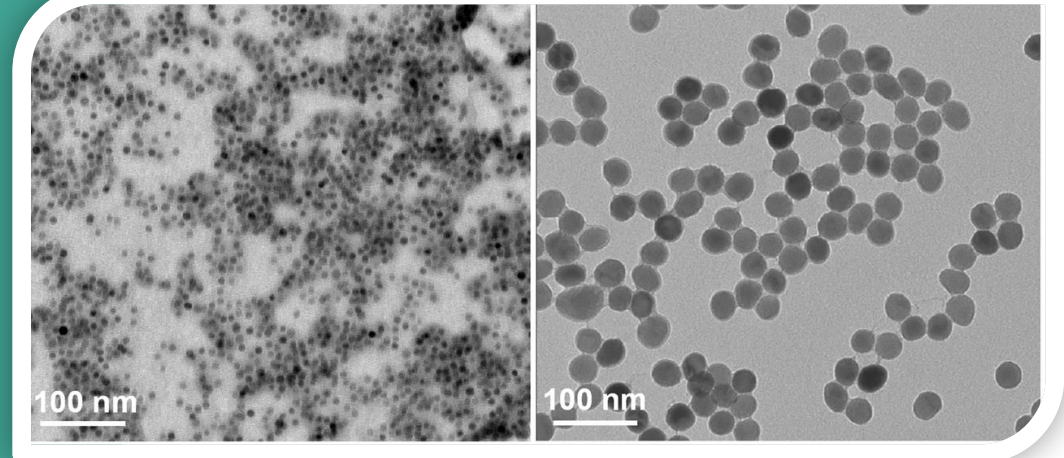
Physicochemical
properties of NMs
influencing toxicity

Physicochemical properties of NMs influencing (eco)toxicity

Size

- Small particles tend to be more toxic than larger particles from the same material.

Physicochemical
properties of NMs
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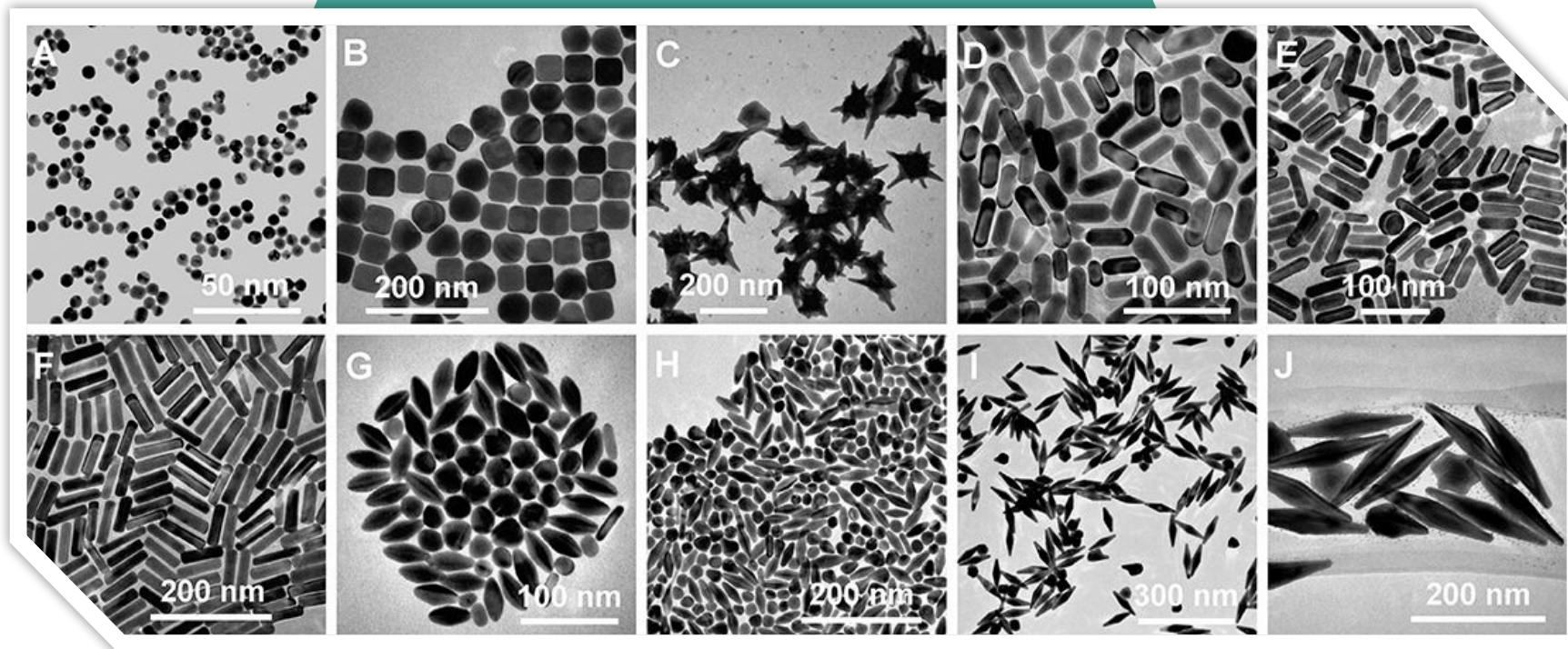


Sci. Rep. 2018, 8, 2082

Physicochemical properties of NMs influencing (eco)toxicity

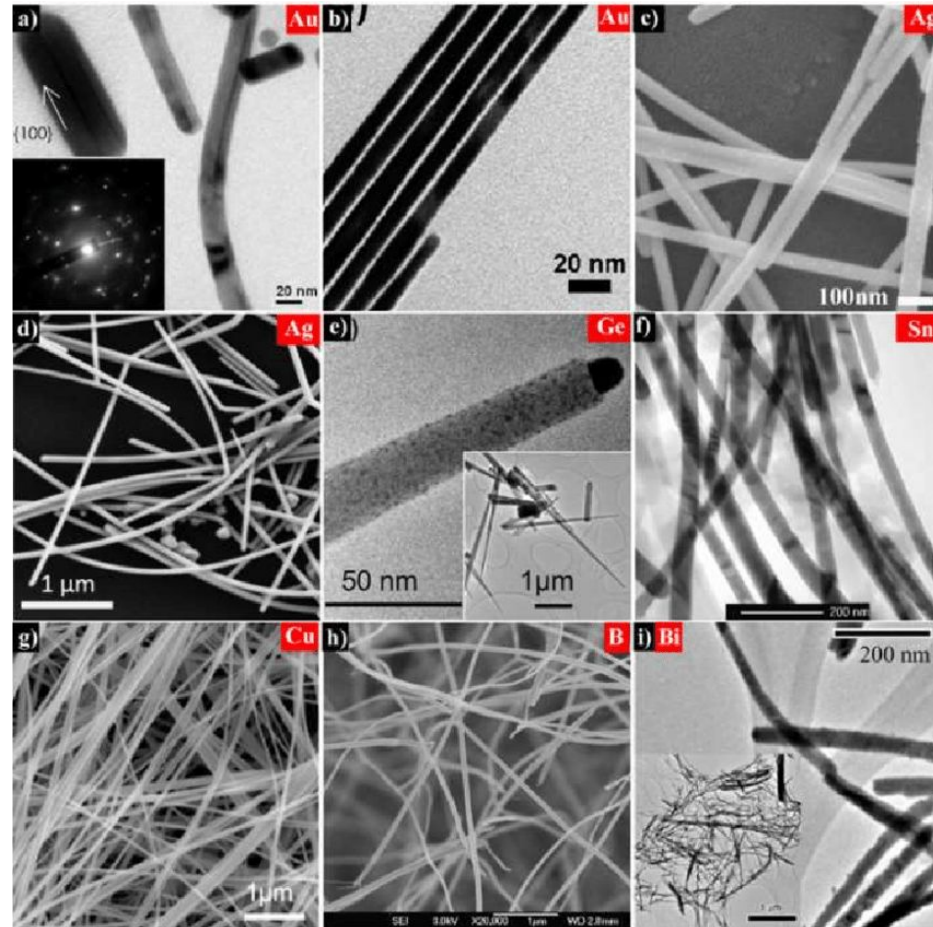
Shape

- Toxic interaction with cells can be enhanced due to the shape of the NMs.



Front. Chem. 2019, 7:167.

Physicochemical properties of NMs influencing (eco)toxicity

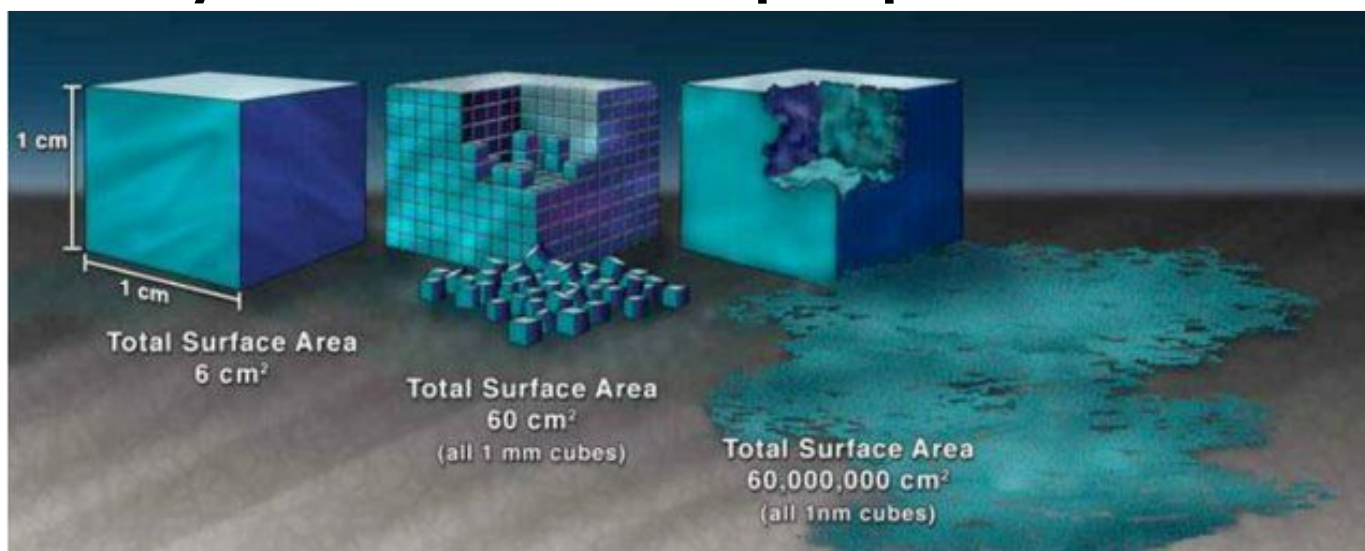


Aspect ratio

- Fibers tend to be more toxic than particles.

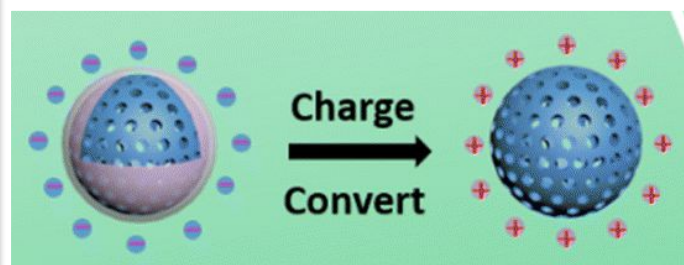
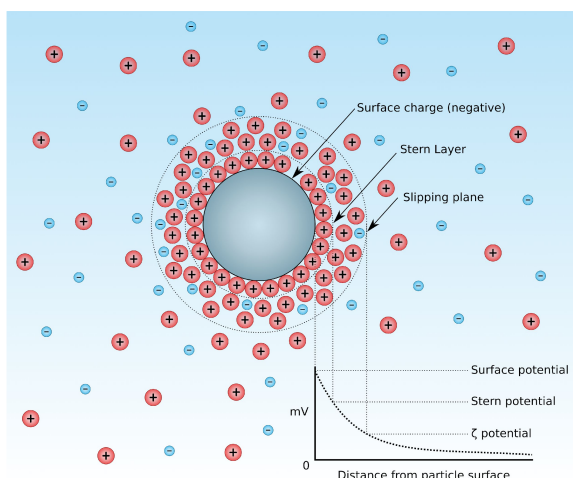
Chapter: Electrical properties of nanowires and nanofibers.
Published in the Book Handbook of nanofibers. Copyright
Information Springer Nature Switzerland AG 2019.

Physicochemical properties of NMs influencing (eco)toxicity



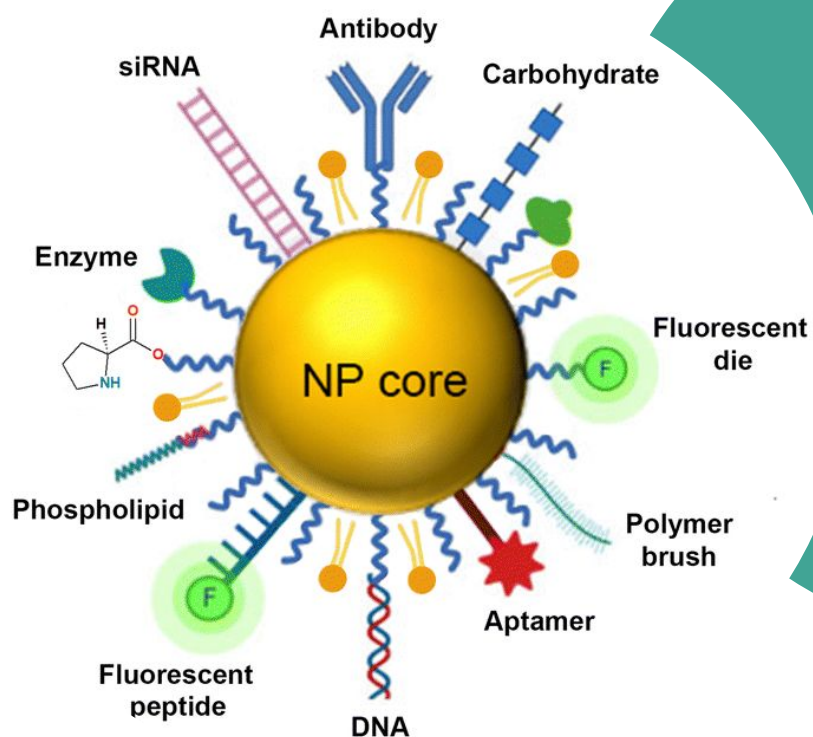
Surface area and surface charge

- The reactivity of NMs grows with increasing surface area (more sites for chemical reactions/interactions are provided), which influences the toxicity of the materials.
- Surface charge affects the interaction of NMs with cell membranes.



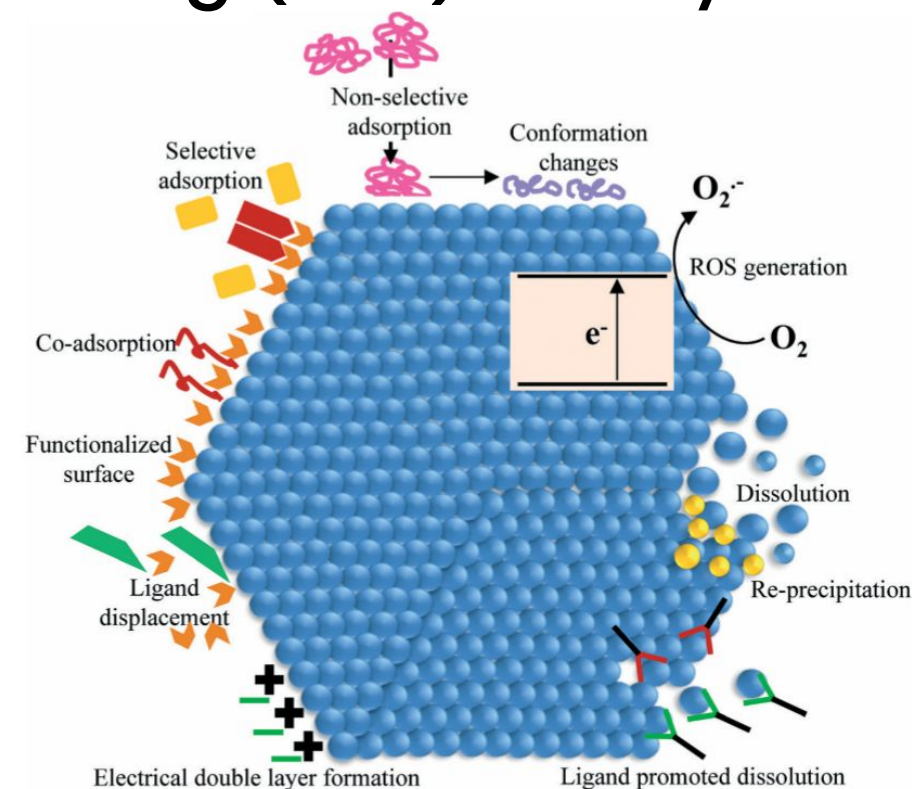
Nanoscale, 2023, 15, 13202-13223

Physicochemical properties of NMs influencing (eco)toxicity



Chem. Soc. Rev., 2023, 52, 2573-2595

Physicochemical properties of NMs influencing toxicity



Environ. Sci. Nano 2015, 2:429

Surface chemistry and functionalization

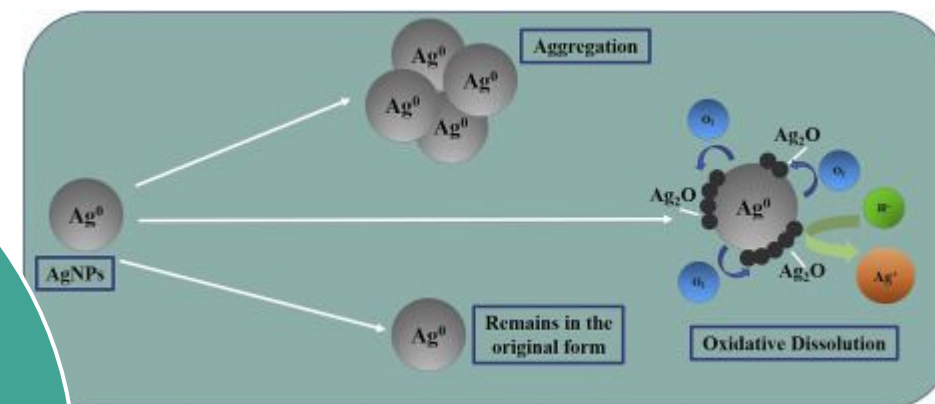
- The chemical composition of the surface and the presence of functional groups may alter NMs i.e., reactivity, solubility, interaction with biological systems, affecting their toxicity.

Physicochemical properties of NMs influencing (eco)toxicity

Physicochemical
properties of NMs
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Solubility and dispersion

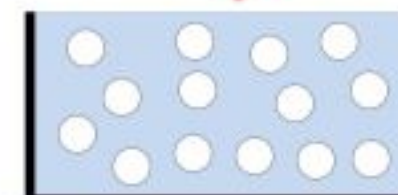
- The ability of NMs to dissolve or remain dispersed in biological fluids affect their bioavailability, distribution, and potential for accumulation in organs.



Chemosphere, 2019, Volume 216, Pages 297-305



Poorly-dispersed TiO_2



Well-dispersed TiO_2

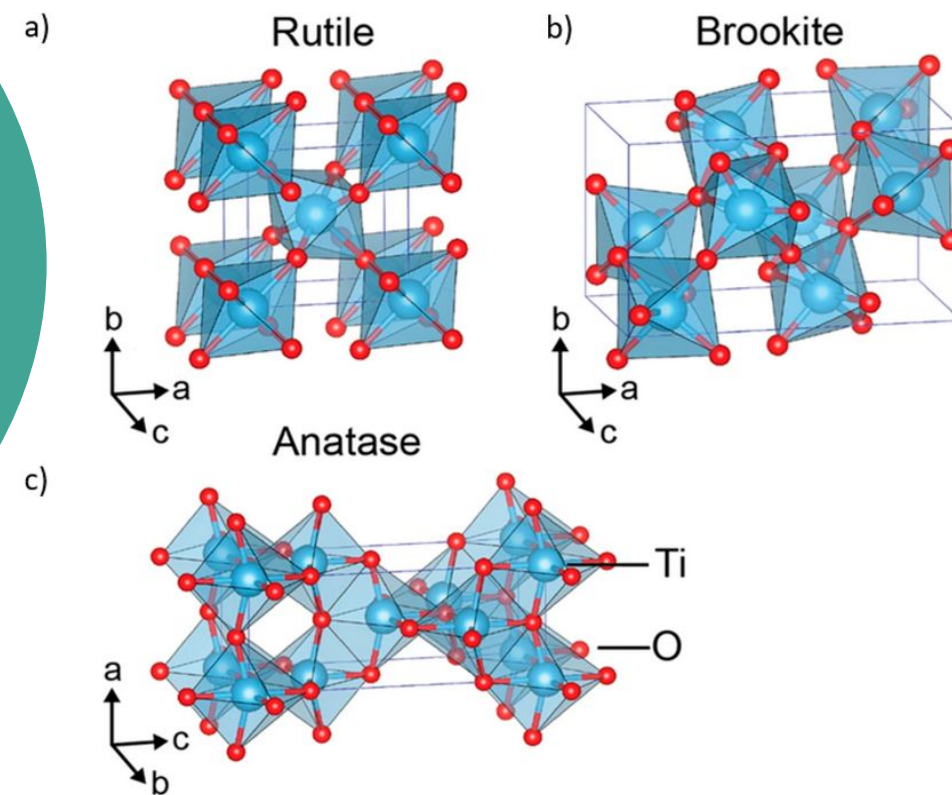
Applied Surface Science, 2015,
Volume 357, Part B, 1658-1665

Physicochemical properties of NMs influencing (eco)toxicity

Chemical Composition and Crystalline Structure

- Toxicity depends on the chemistry (e.g., inherent toxicity of metals) and the crystalline form of the NMs.

Physicochemical properties of NMs influencing toxicity



Nanomaterials 2020, 10(6):1121

Physicochemical properties of NMs influencing (eco)toxicity

Size

- Small particles tend to be more toxic than larger particles from the same material.

Shape

- Toxic interaction with cells can be enhanced due to the shape of the NMs.

Aspect ratio

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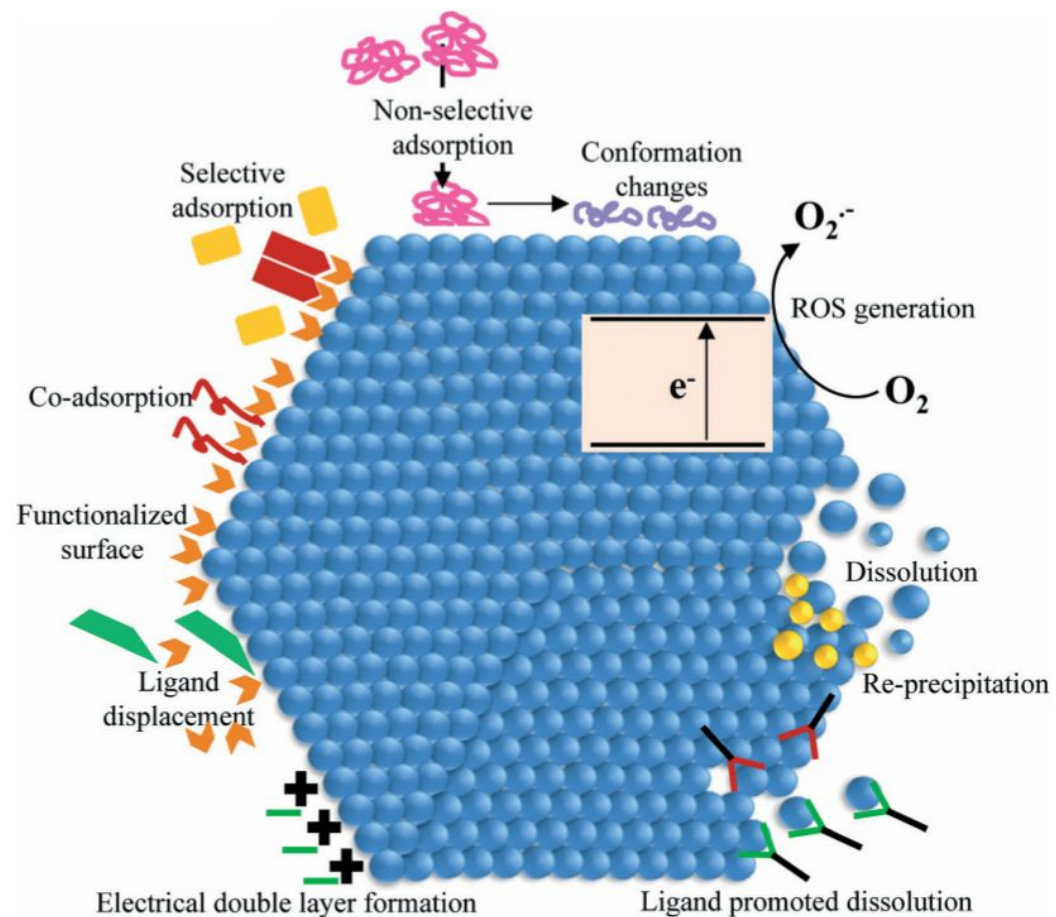
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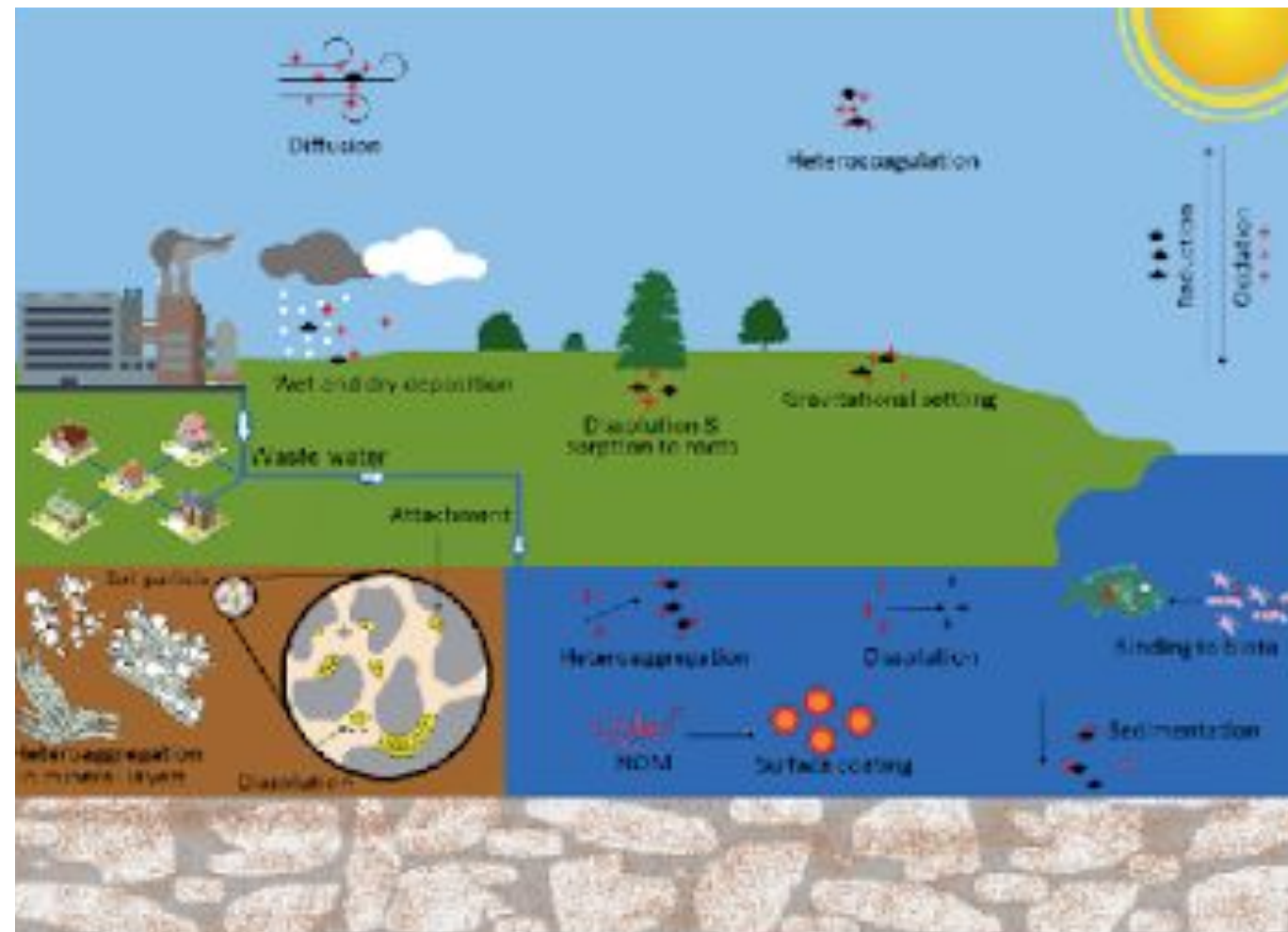
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Environmental fate and behaviour

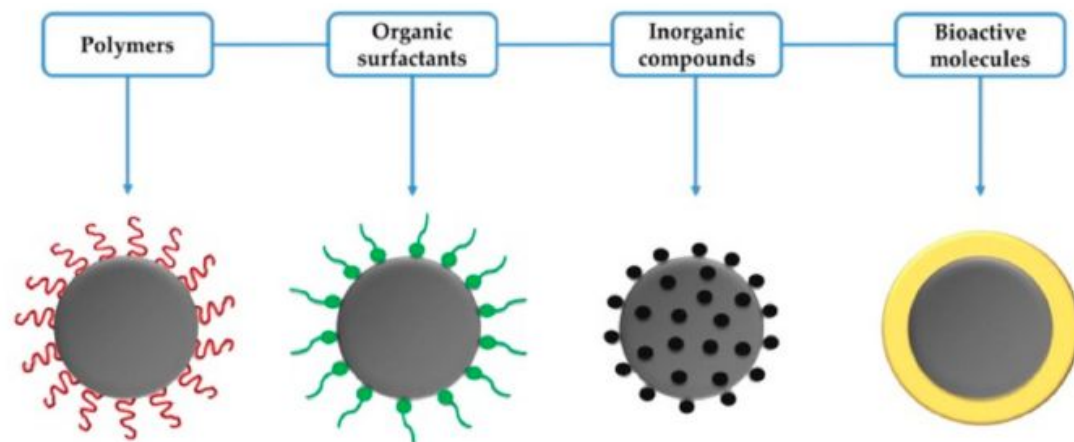


Environ. Sci. Nano 2015, 2:429

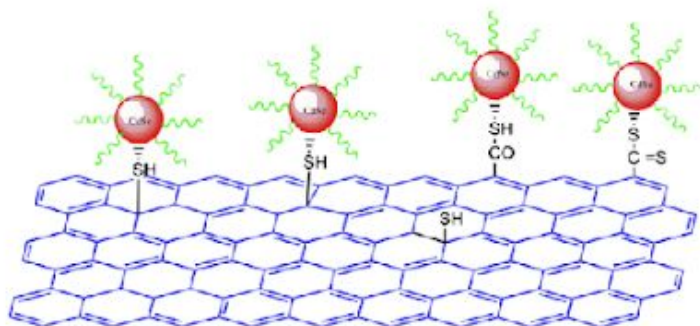


Environment International 2020, 130, 105646

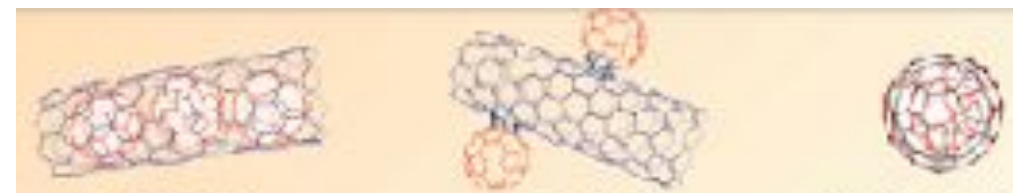
Advanced materials (AdMa)



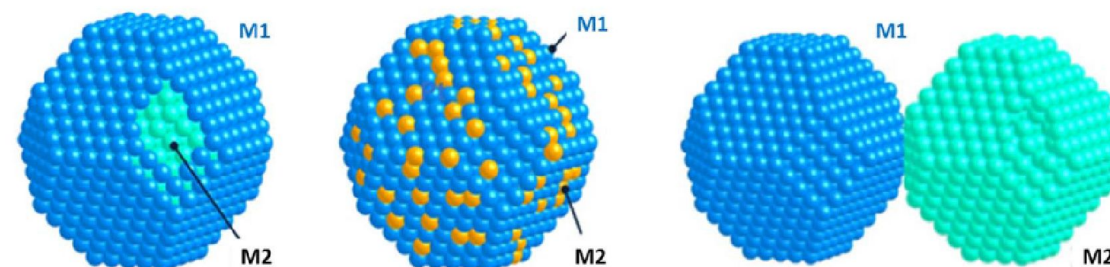
Pharmaceutics 2019, 11, 601



Chemical Engineering Journal 2013, 231,146–154

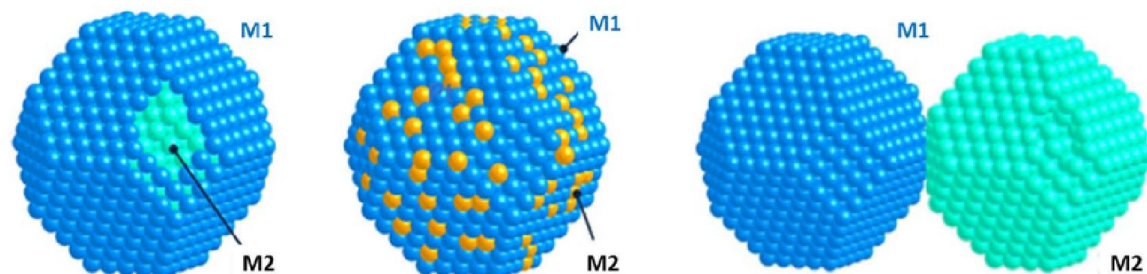


Environ. Sci.: Nano 2015, 2, 11–18

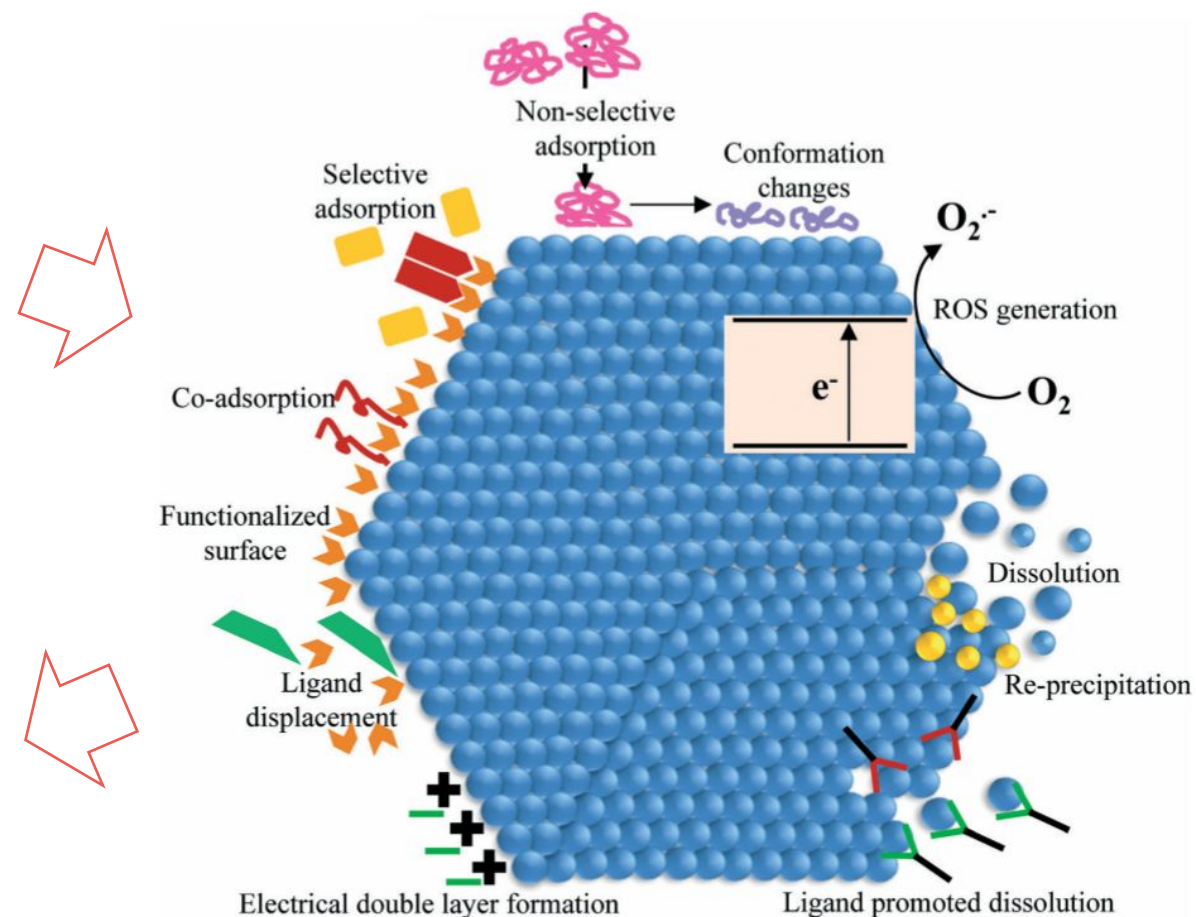
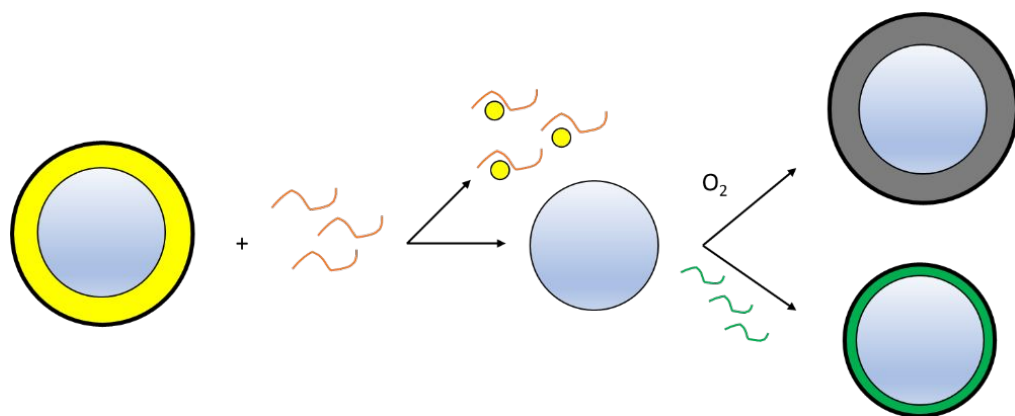


J. Electrochem. Soc. 2018, 165, 3222

Physicochemical properties of AdMa influencing (eco)toxicity



J. Electrochem. Soc. 2018, 165, 3222

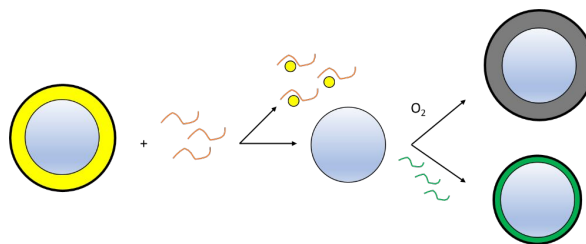


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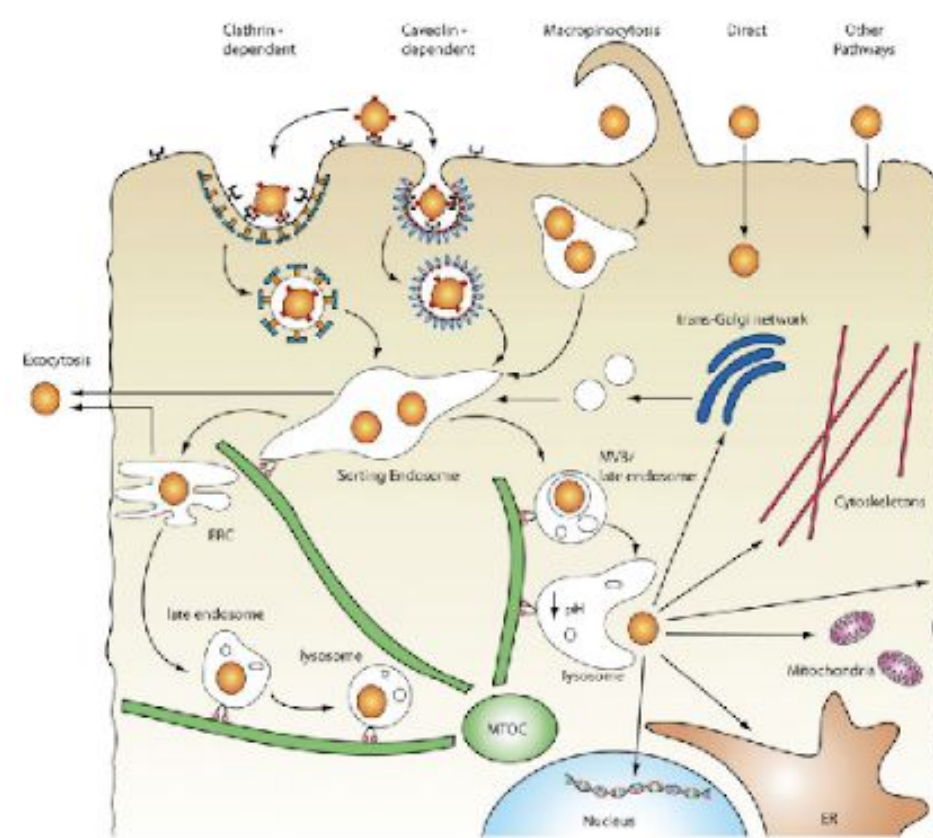
Physicochemical properties of AdMa influencing (eco)toxicity



Changes in toxicity



Different components can reach the same site at the same time and show different toxicological mechanism of action



Nanomaterials 2019, 9, 1719

“Mixture” effects may occur

AdMa embedded in a matrix



AdMa embedded in a matrix



Selection of suitable analytical
methods for advanced material
characterization

