CEINT's NanoPHEAT Project

Integrating Exposure and Toxicity Data to Build Risk Forecasting Tools

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Mark Wiesner

Duke UNIVERSITY

CONSUMER PRODUCT SAFETY COMMISSION UNITED STATES

NIST National Institute of Standards and Technology U.S. Department of Commerce

U.S. ARMY ENGINEER RESEARCH AND DEVELOPMENT CENTER ERDC

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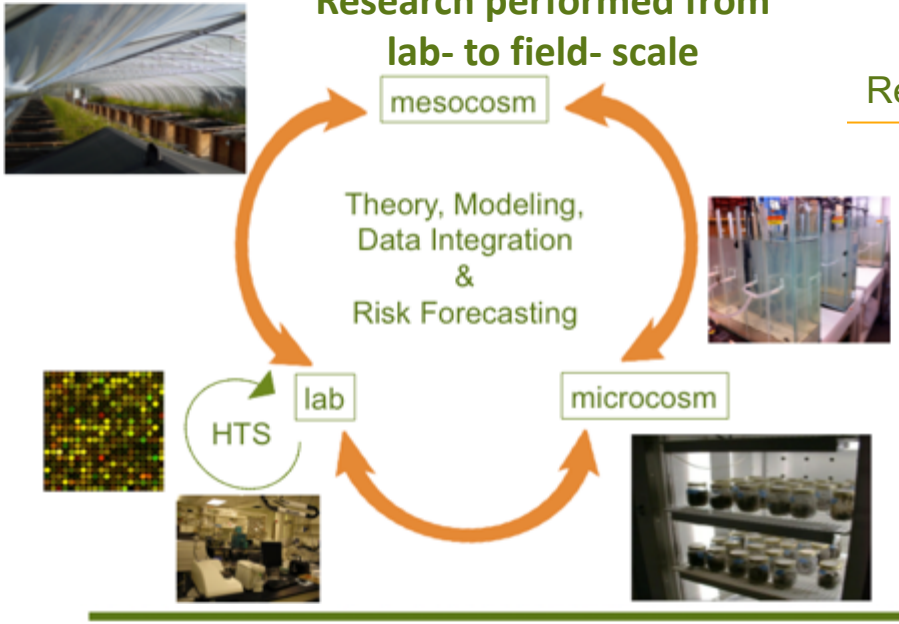
Center for the Environmental Implications of NanoTechnology

- To elucidate the general principles that determine ***nanomaterial behavior*** in the environment
- To identify data and metadata necessary to support ***forecasts of exposure potential***, bioaccumulation, and bioactivity
- To identify key ***measurement assays*** that are predictive of outcomes of interest



Research teams:

1. Exposure, transport and transformation
2. Cellular and organismal impacts
3. Ecosystem-level impacts
4. Nanomaterial fabrication and characterization
5. Natural, incidental nanomaterials and detection in complex systems
6. Modeling, Risk Forecasting, Materials Informatics

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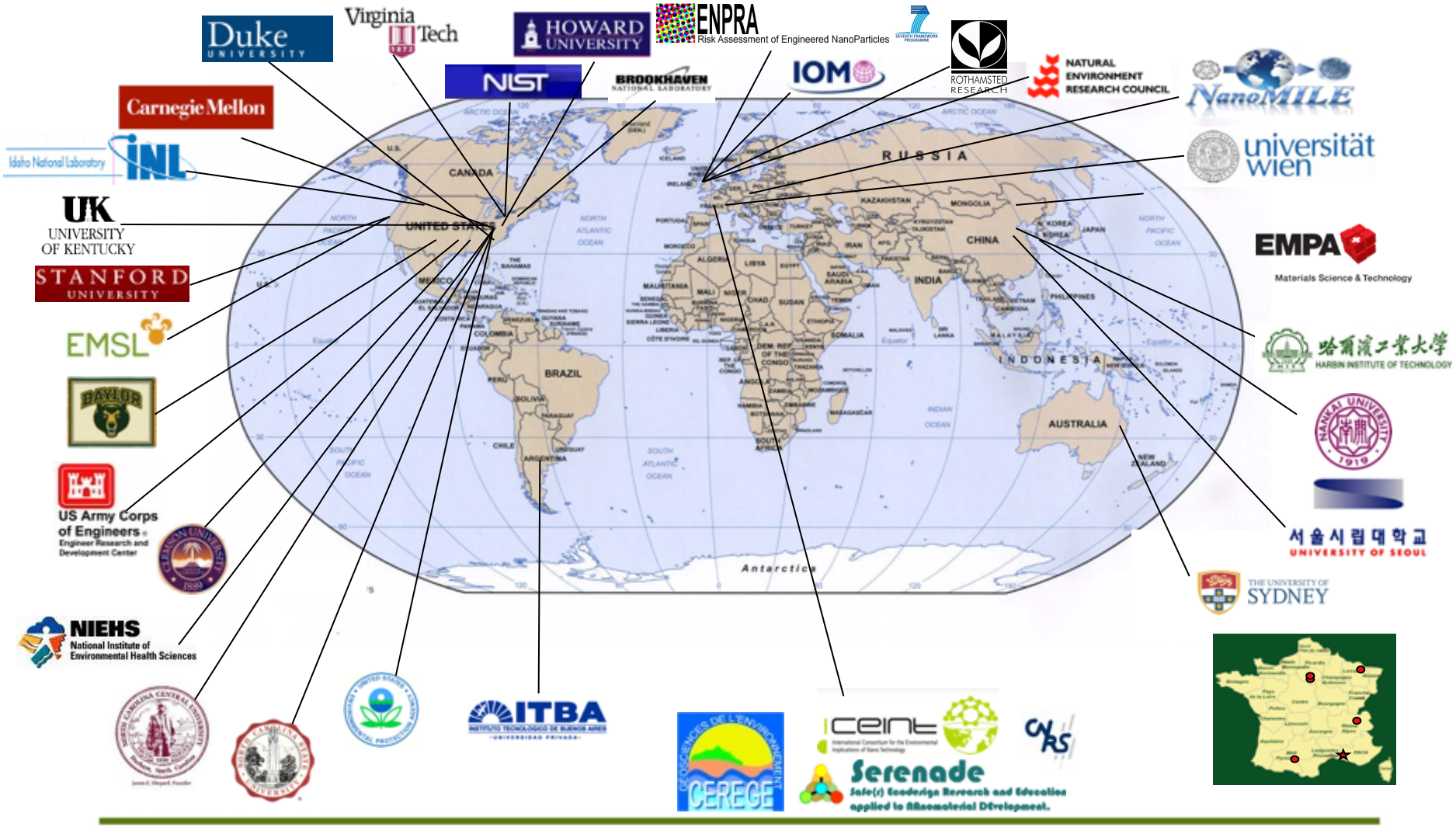

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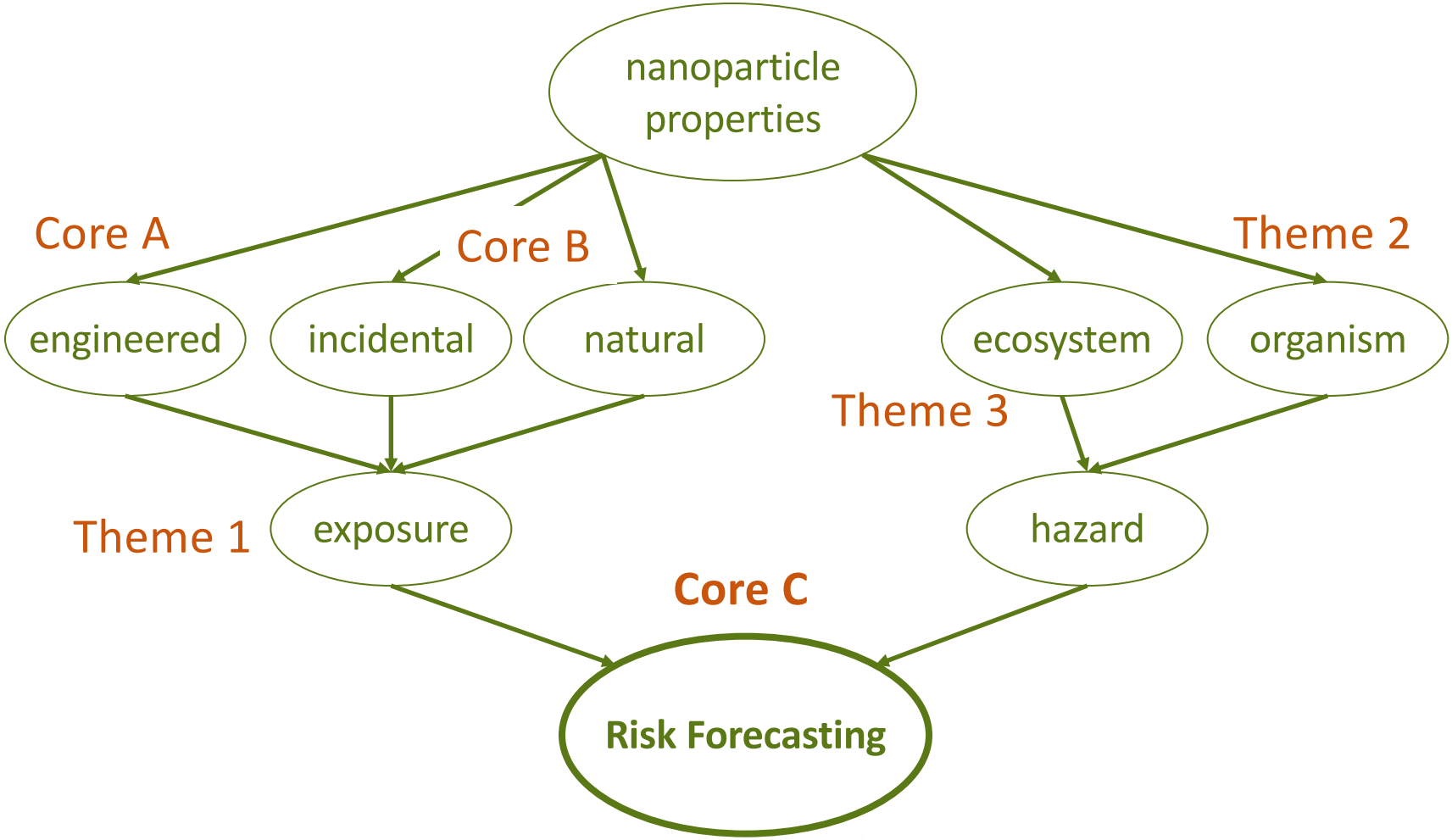
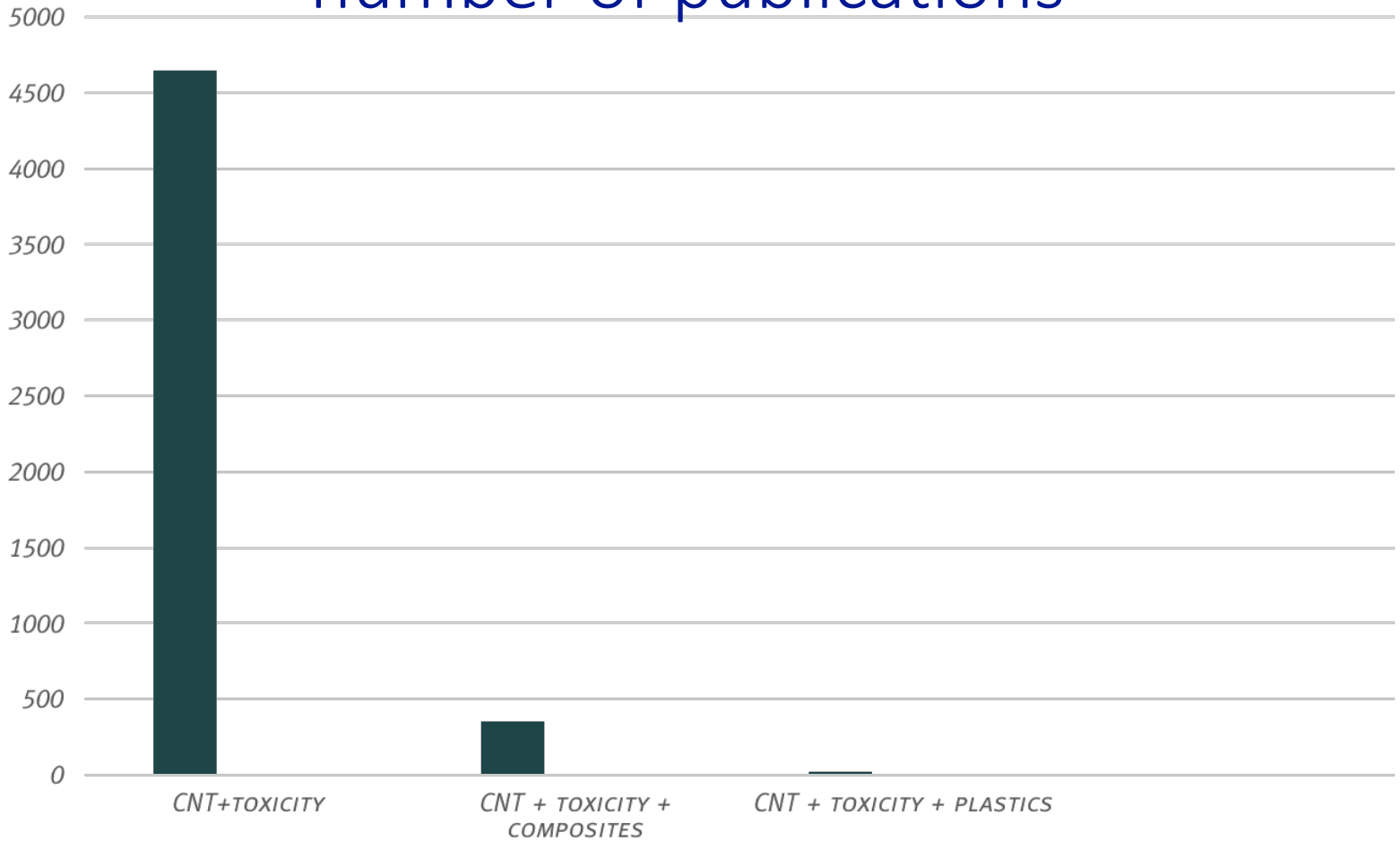


Pristine vs nanocomposites- comparison of number of publications

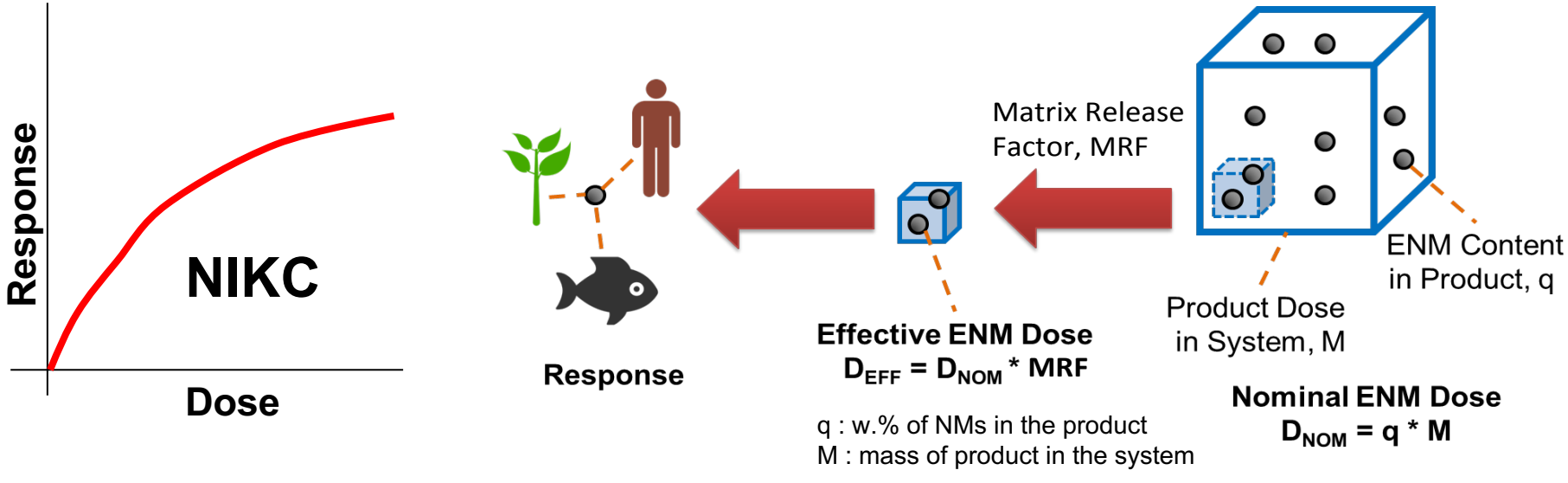


NanoPHEAT

(Nano Product Hazard and Exposure Assessment Tool)

&

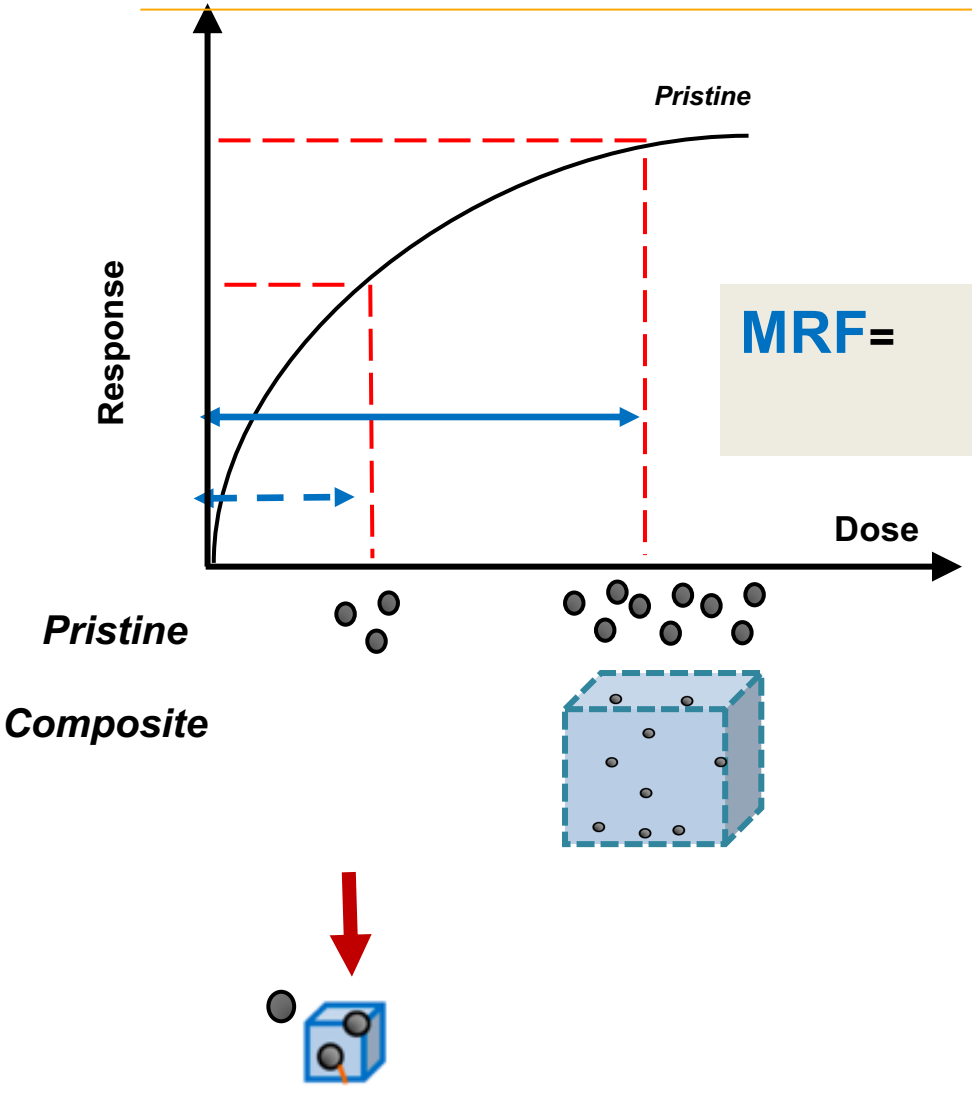
The NIKC (NanoInformatics Knowledge Commons)



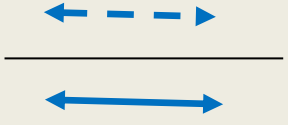
Realism & Generalizability + Tool for Immediate Guidance & Modular Expansion

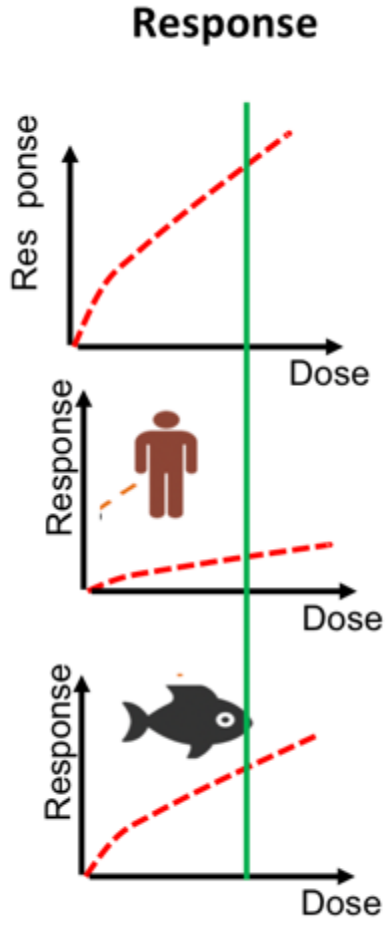
- Realistic matrices and well characterized release scenarios
- Leverage existing data
- Incorporate emerging product-specific data

NanoPHEAT Model + Matrix Release Factor (MRF)

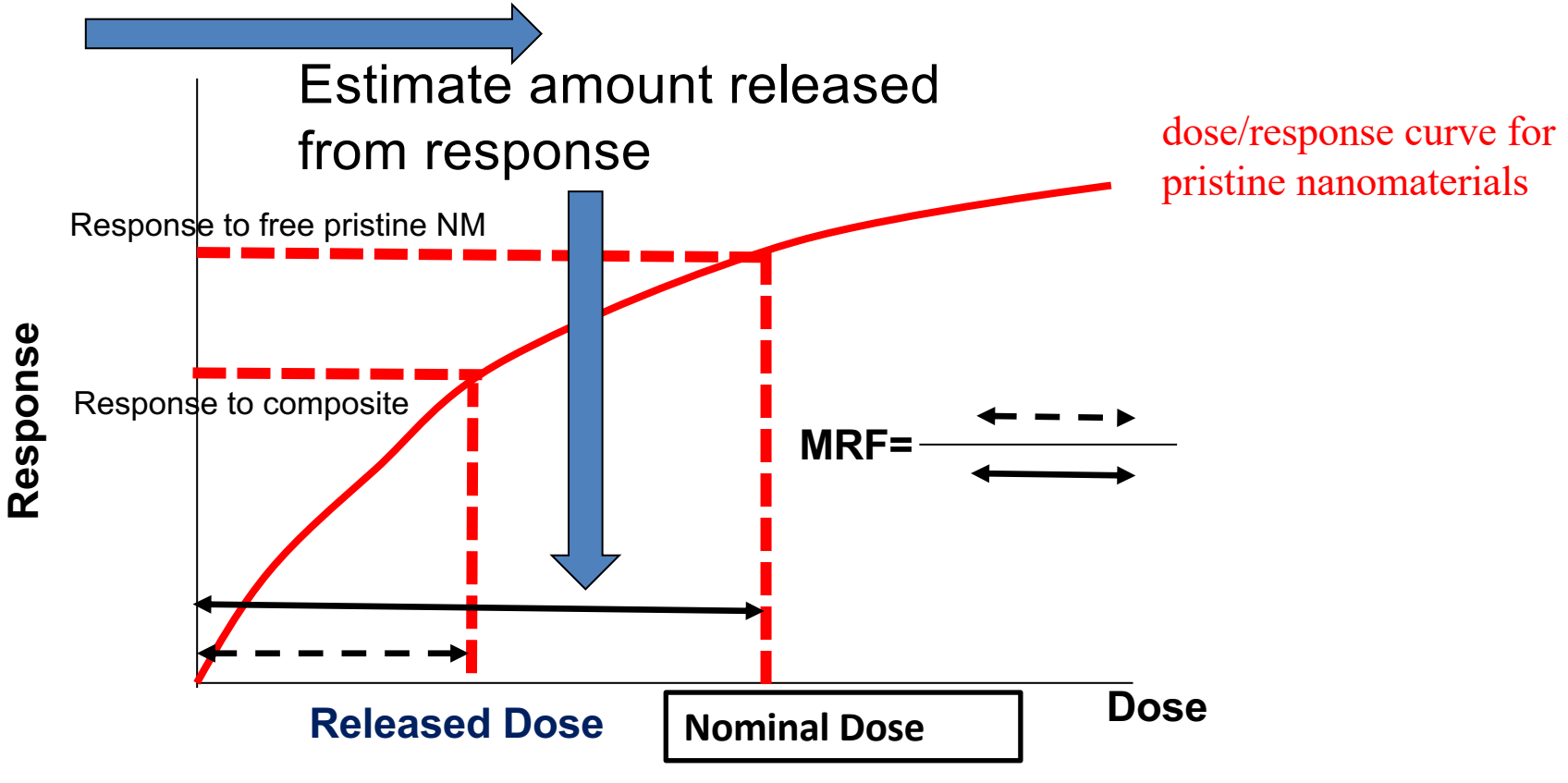


MRF=





Interpreting the Matrix Release Factor (MRF)



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NIKC Database

NanoInformatics Knowledge Commons

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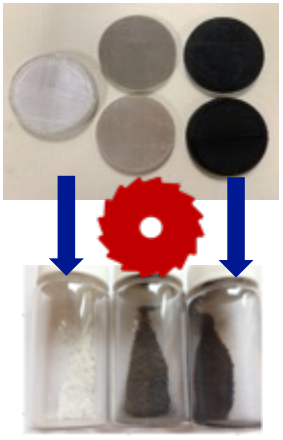
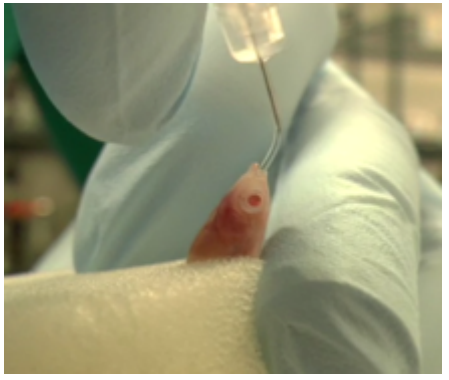
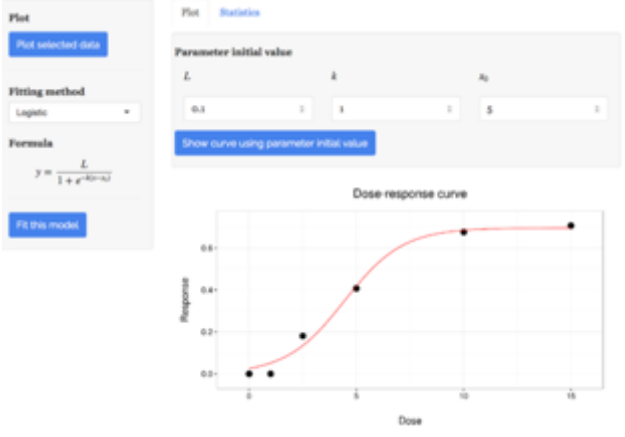


Toxicity Studies



NanoPHEAT Tool



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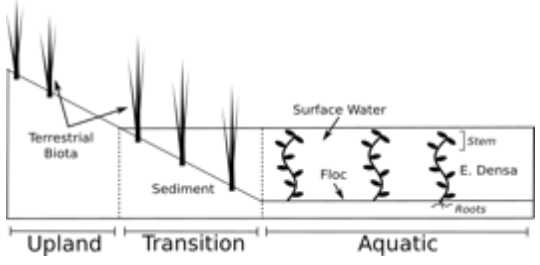
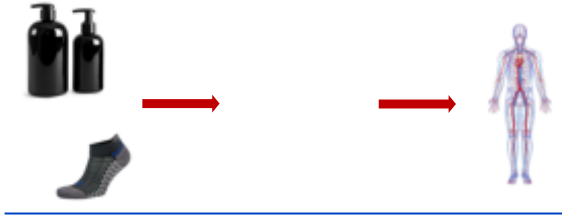
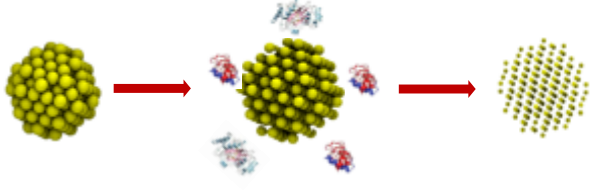
Uses of the NIKC Database Structure

Shared Resources







NanoInformatics Knowledge Commons

Collaborators

Serenade

Cerege
CENTRE EUROPÉEN DE RECHERCHE ET D'ENSEIGNEMENT DES GÉOSCIENCES DE L'ENVIRONNEMENT

NanoFASE

U.S.ARMY

CONSUMER PRODUCT SAFETY COMMISSION

NIST National Institute of Standards and Technology U.S. Department of Commerce

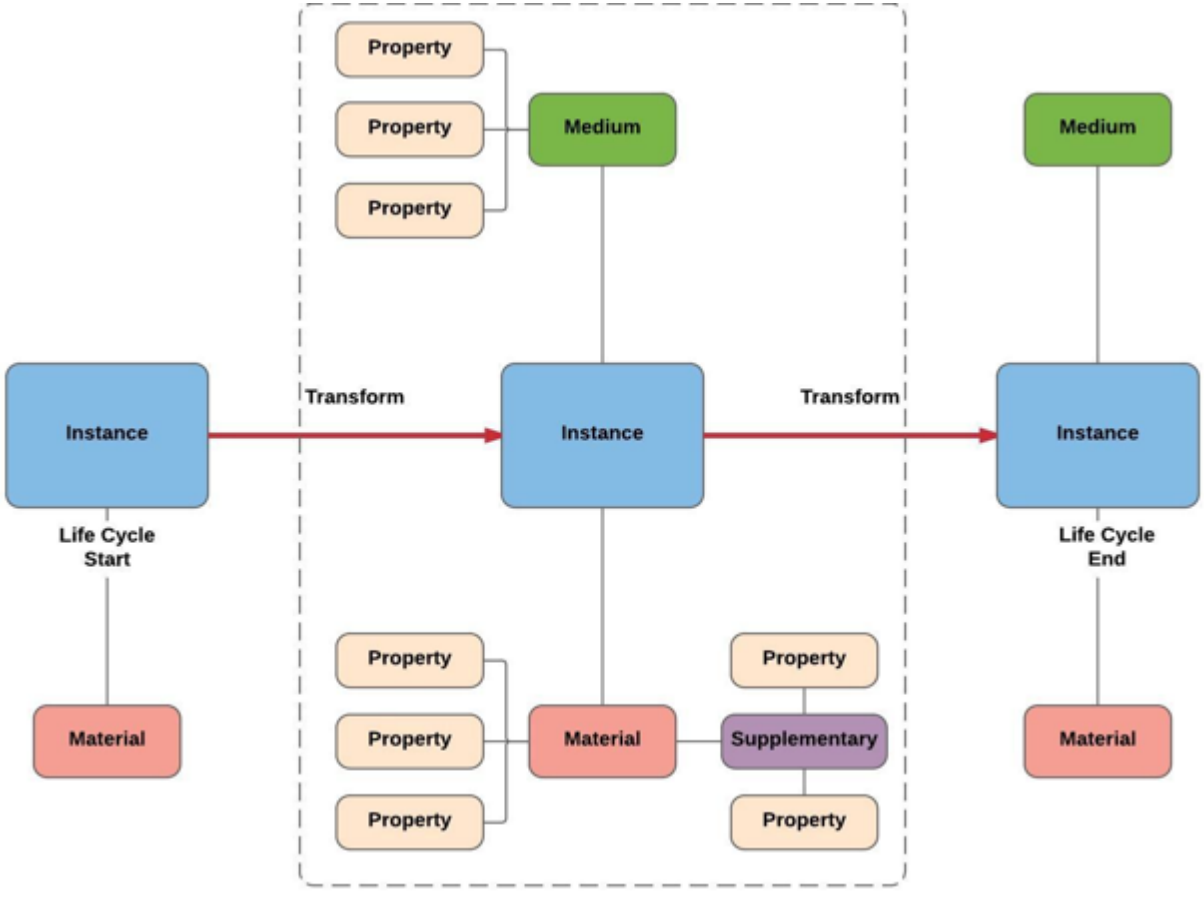
The Center for Sustainable Nanotechnology

NanoFASE

NanoCommons
Nano-Knowledge Community

eNM eNanoMapper

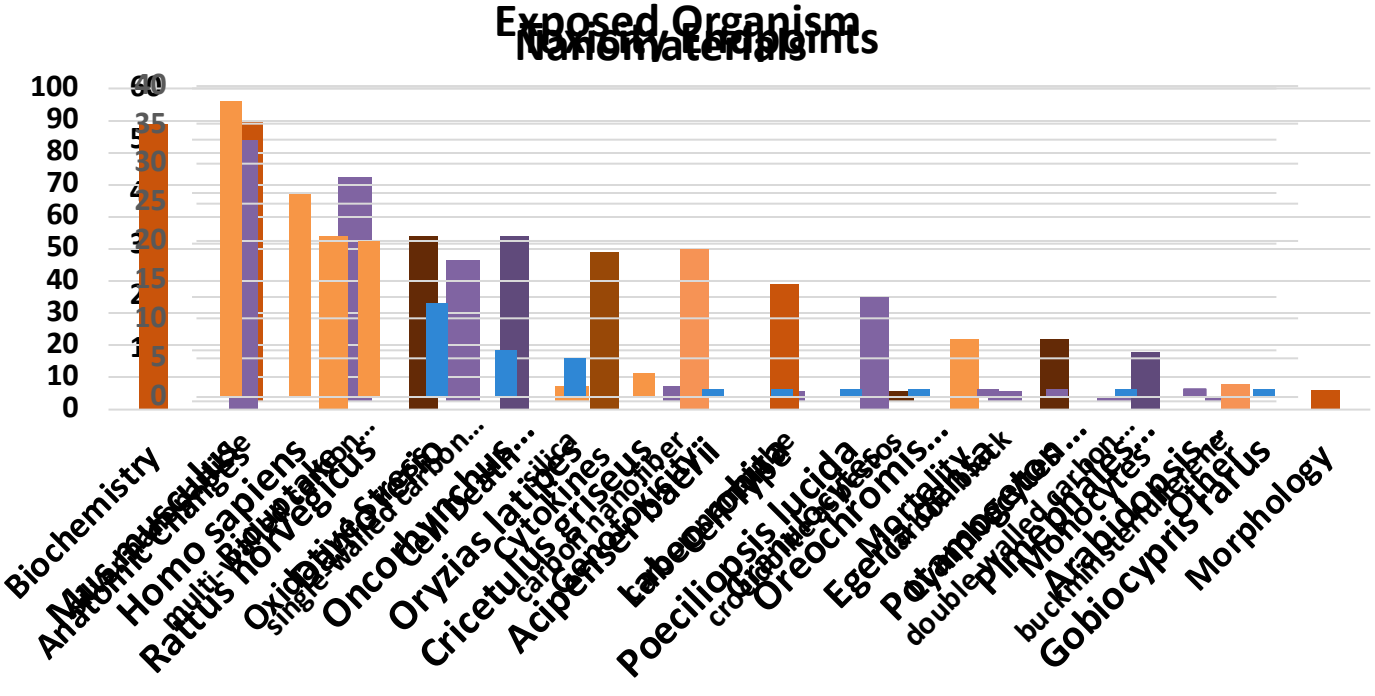
NIKC Instance Organizational Structure



NIKC Database Accomplishments

Creating dose-response curves for NanoPHEAT Tool using pristine data

- Curated 120 peer-reviewed papers of toxicity responses from pristine nanomaterials



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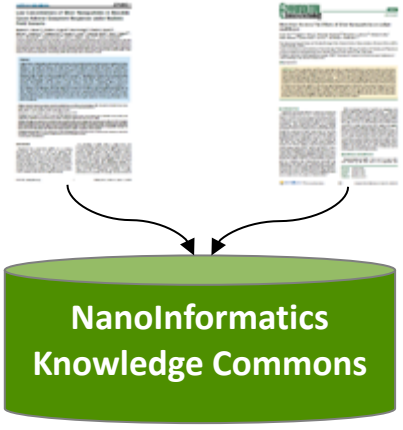
NIKC Database



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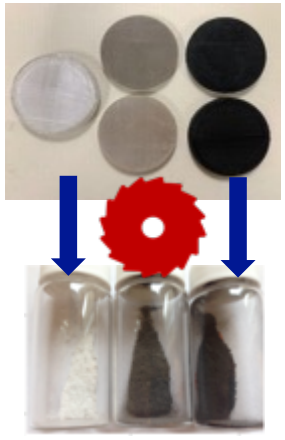
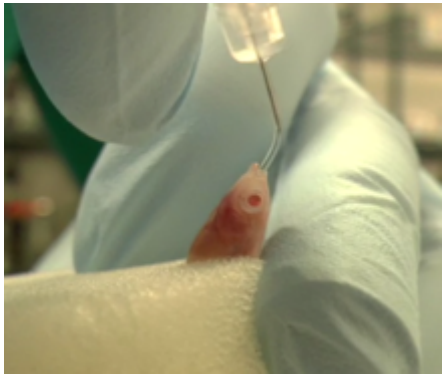
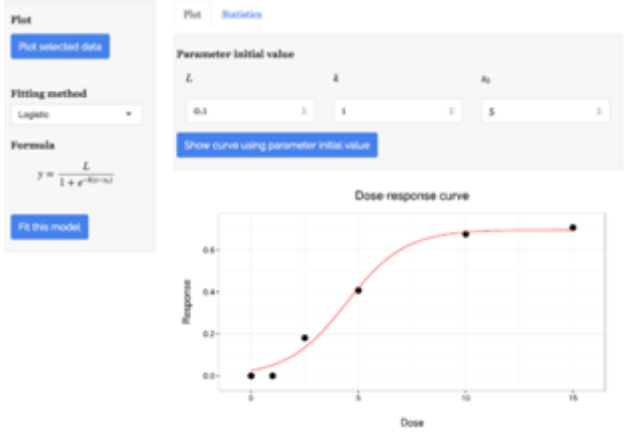


Toxicity Studies



NanoPHEAT Tool



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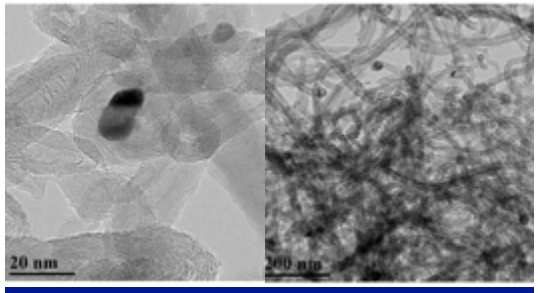
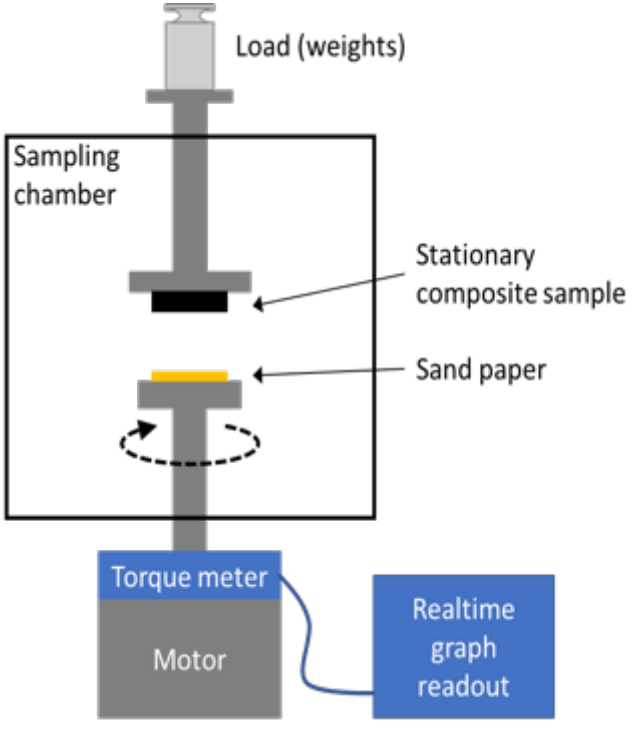
Nanomaterials in Consumer Products

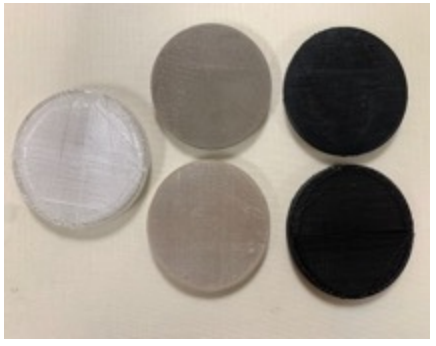
Nanomaterials are added into Polymer Products to Enhance Features

PETG Products containing MWCNTs & Ag NPs



Ag NPs MWCNTs





https://fr.aliexpress.com/

https://owensmanagement.com.au/nano-coating-technology/

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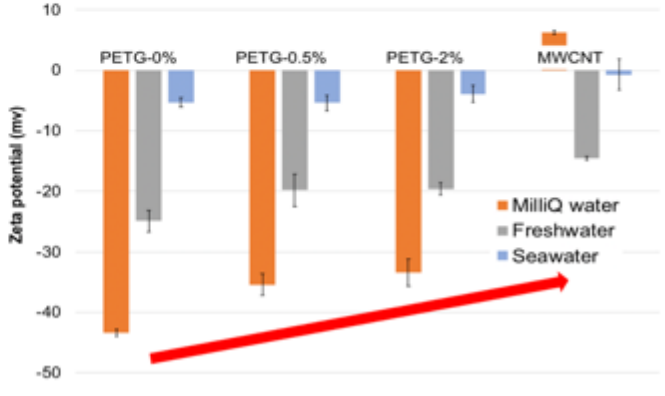
MWCNT Composite Particle Changes

- Mechanical properties

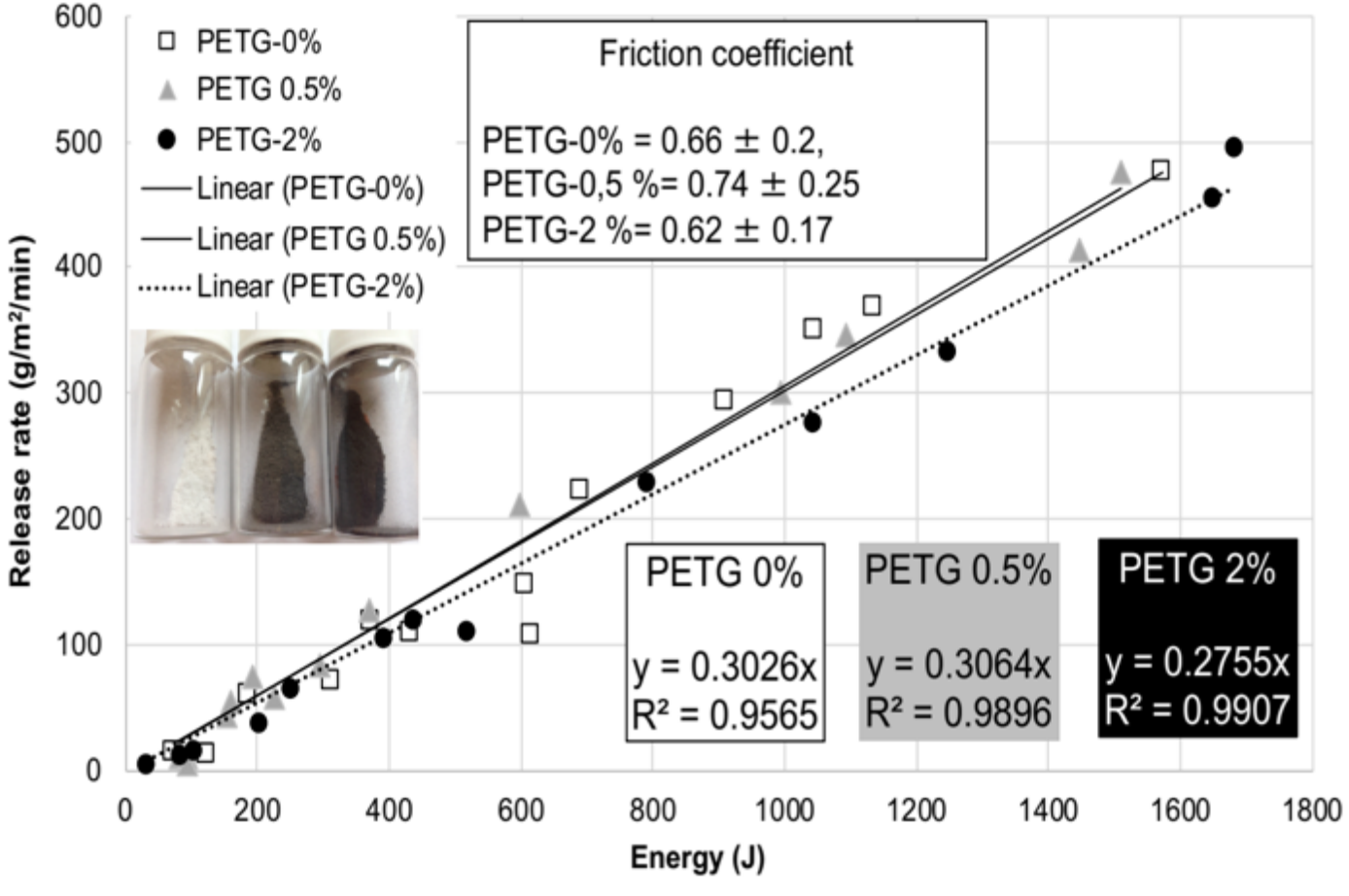
Sample name	Ultimate Tensile Strength	Young's Modulus	Glass transition temperature °C
PETG 0%	43.54 ± 1.43 MPa	1.53 ± 0.09 GPa	83.71
PETG 0.5%	43.63 ± 1.09 MPa	1.74 ± 0.03 GPa	84.09
PETG 2%	49.70 ± 1.80 MPa	1.82 ± 0.18 GPa	84.29

- **Hydrophobicity**

  - PETG-0 w.%= 65.2°
  - PETG-0.5 w.%= 72.2°
  - PETG-2 w.%= 86.6°



Release Rate of Microplastic + MWCNT



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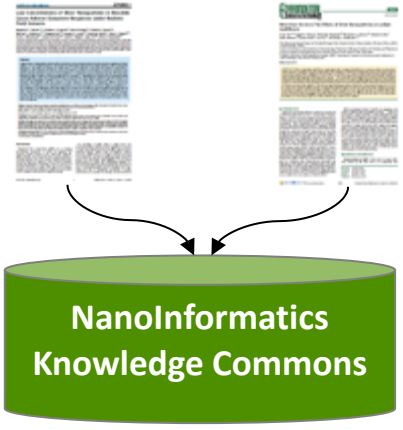

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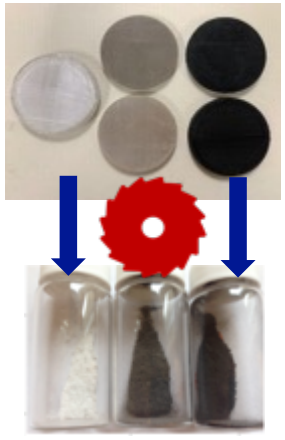

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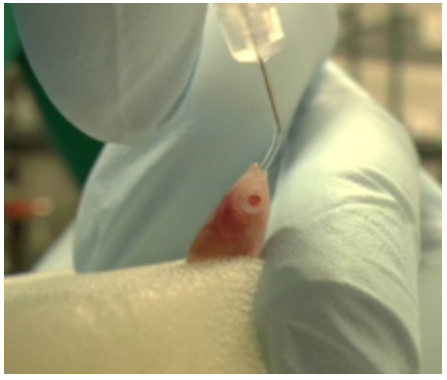

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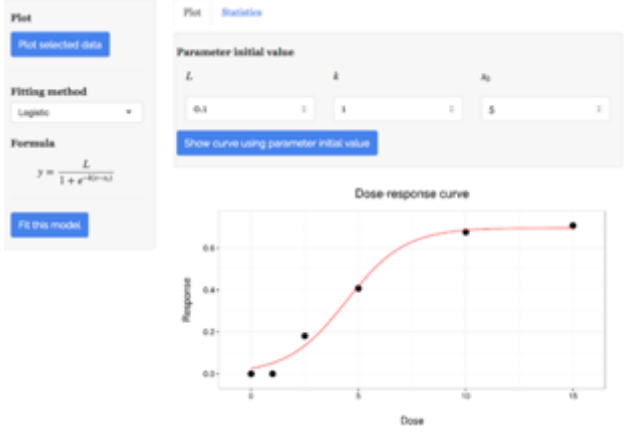

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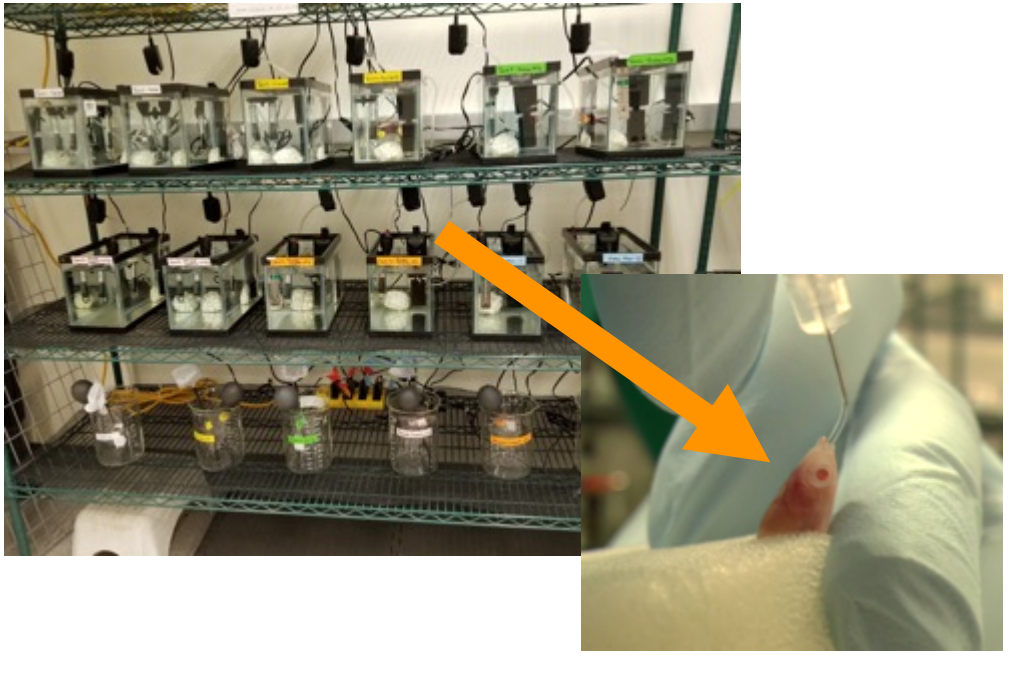
Japanese Medaka (Oryzias latipes)

- Aquatic model organism for toxicity studies:
  - Amenable to the laboratory
    - Small (3-4cm)
    - Mature within 8-12 weeks
  - Anatomy well described

Quintet mutant medaka

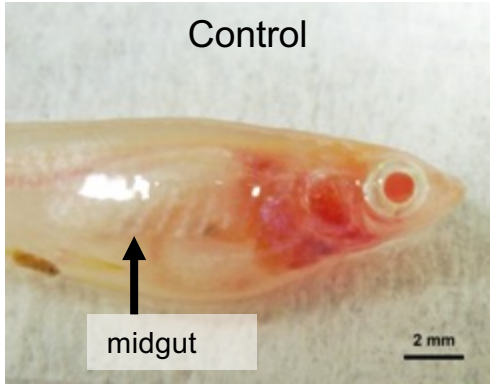


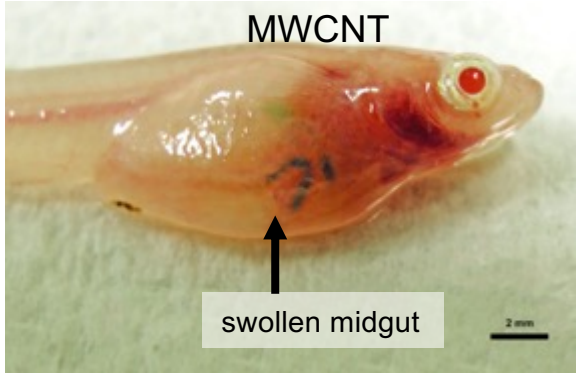
Dose Response Pristine NM	Toxicity of Matrix Effect
200-1000 ppm MWCNT	1000 ppm MWCNT held constant changing amount of plastic

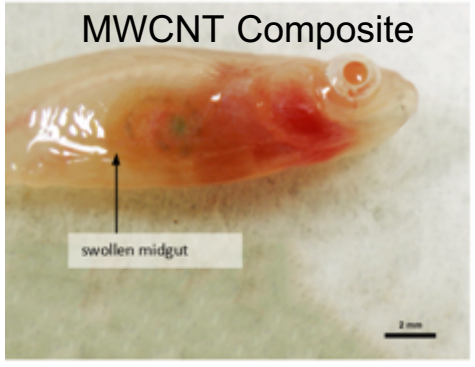
7 oral gavages over 14 days

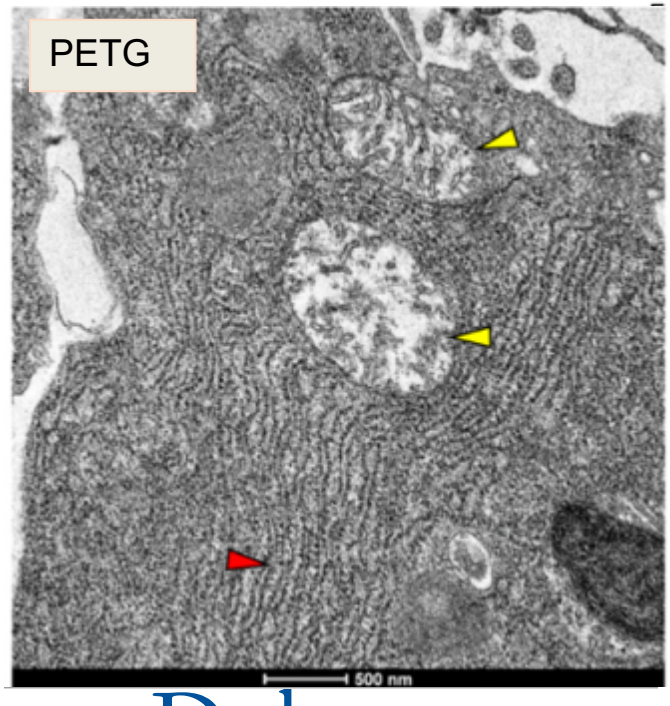
- Fish fasted day before gavage
- Material suspended in 10ul of distilled water = 1 dose

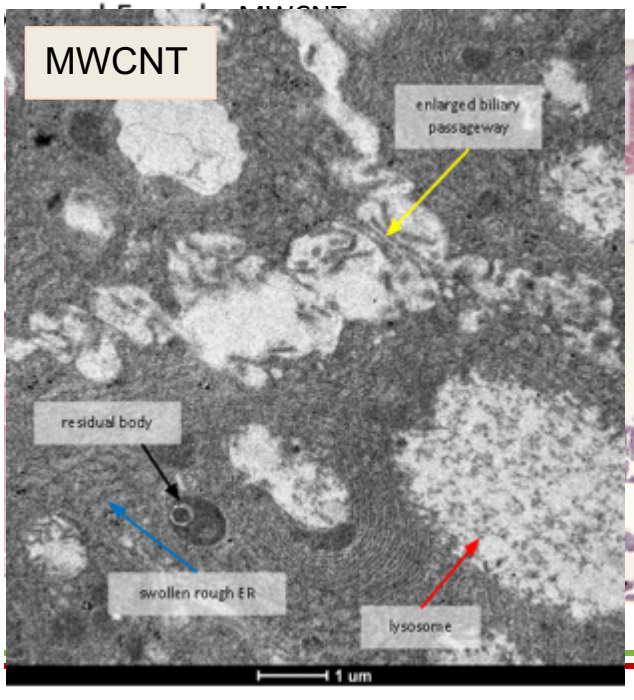
Toxicity Overview for Pristine NM vs. Composites

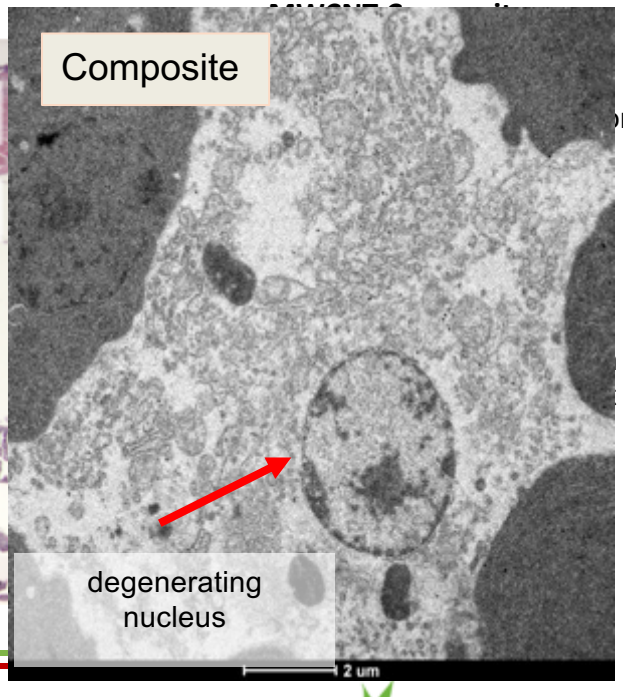












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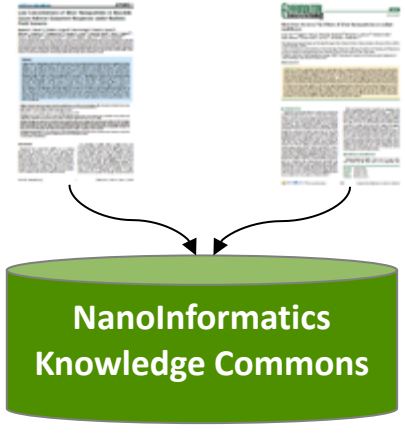

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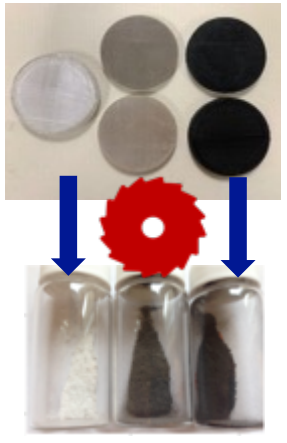
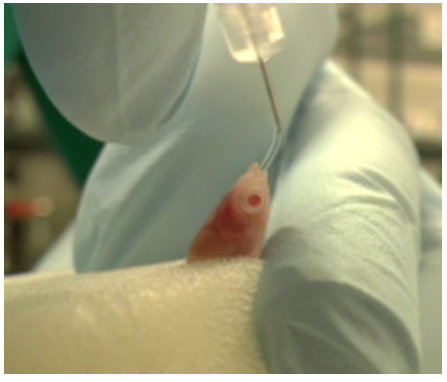


Toxicity Studies



NanoPHEAT Tool

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Jaleesia Amos Guided Walkthrough

NANOPHEAT TOOL DEMONSTRATION

What we have learned

NIKC – Instance Organizational Structure allows us to follow the nanomaterial transformations over time, potential enabling more in-depth analysis of curated data.

Nanomaterial-matrix composites do not behave in the same way as pristine nanomaterial in product use.

There are systemic responses through oral exposure pathway from particles released from the NM composites that are unique from the pristine NMs and the matrix.

Thank You!

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Team	Participants
Leadership Team	Mark Wiesner (PI) Christine Hendren (co-PI) Treye Thomas (CPSC) Alan Kennedy (US-Army Corps of Engineers)
Curation Team	Jaleesia Amos (Duke) Zhao Zhang (Duke)
NanoPHEAT App Team	Yuan Tian (Duke) Nathan Bossa (Duke) Jaleesia Amos (Duke)
Exposure Team	Joana Sipe (Duke) Nathan Bossa (Duke) Keana Scott (NIST) William Berger (Duke)
Toxicology Team	David Hinton (Duke) Melissa Chernick (Duke)
US-Army Team	Alan Kennedy (US- Army Corps of Engineers) Taylor Rycroft (US- Army Corps of Engineers) Jason Deng (US- Army Corps of Engineers) Igor Linkov (US- Army Corps of Engineers)