The CEINT Informatics Knowledge Commons

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CEINT
Center for the Environmental Implications of NanoTechnology

The CEINT Informatics Knowledge Commons design reflects the analytical needs defined by the dual aspects of the CEINT Mission:

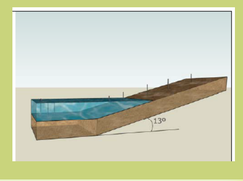
- To elucidate general principles that determine nanomaterial behavior in the environment → *CEINT IKC must support fundamental mechanistic investigations*
- To translate this knowledge into models to forecast risk and to provide guidance in assessing existing and future concerns surrounding the environmental implications of engineered nanomaterials. → *CEINT IKC must support near-term risk-based decisions*

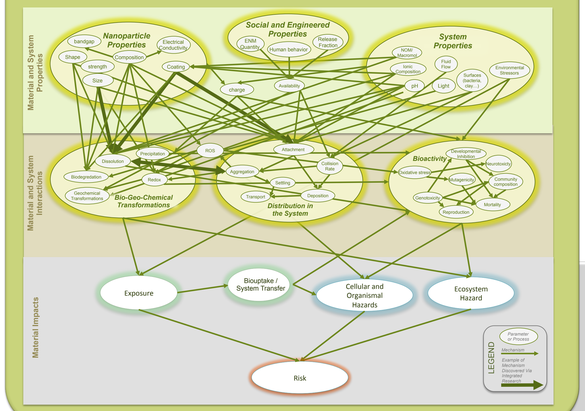
CEINT Informatics Knowledge Commons Objectives

- Develop an integrated database and associated visualization tools that are accessible to CEINT researchers, who can analyze their collective data and utilize tools to visualize their own results integrated with the work of their colleagues and with relevant literature.
- The current CEINT IKC is designed to support curation of data and development of queries at a variety of detail levels in pursuit of targeted research questions for the nanoAg pilot effort. The hypothesis being tested for the pilot study is that functional assay parameters can be utilized to predict nanomaterial exposure, bioaccumulation, and/or toxic effects in complex systems (mesocosms) and in laboratory studies: Questions:
  - Specific functional assays being investigated: attachment, dissolution, biouptake and transformation
  - Are results of exposure, bioaccumulation, and/or toxic effects experiments in laboratory studies with limited independent variables predictive of results in mesocosms?
  - Working backwards from endpoints of interest (exposure concentrations, bioaccumulation, and toxic effects), are there commonalities between materials that impart the same results? (primary particle size, coating, etc.)
- Facilitate direct researcher interactions with the system
  - System designed and data curated by CEINT Data Integration Team (DIT) in close conjunction with CEINT experimentalists to focus on an initial pilot scope to design a modular curation process that can flexibly analyze data at various levels of granularity (Sample papers 1-20)
  - ½ the curated papers come from CEINT work, ½ from non-CEINT published literature
  - Currently capture consistently curated data either at the calculated value level or can accommodate direct measurement and observation level, in support of deeper data-mining and meta-analyses

Supports Detailed Mechanistic Meta-Analysis

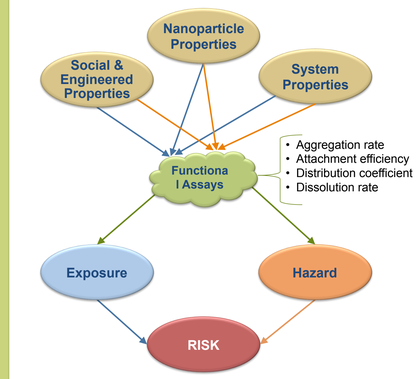
Collect and organize data and meta-data at a level that captures detailed experiments in complex systems to a reproducible level.





Supports Functional Assay Testing for Forecasting of ENM Impacts

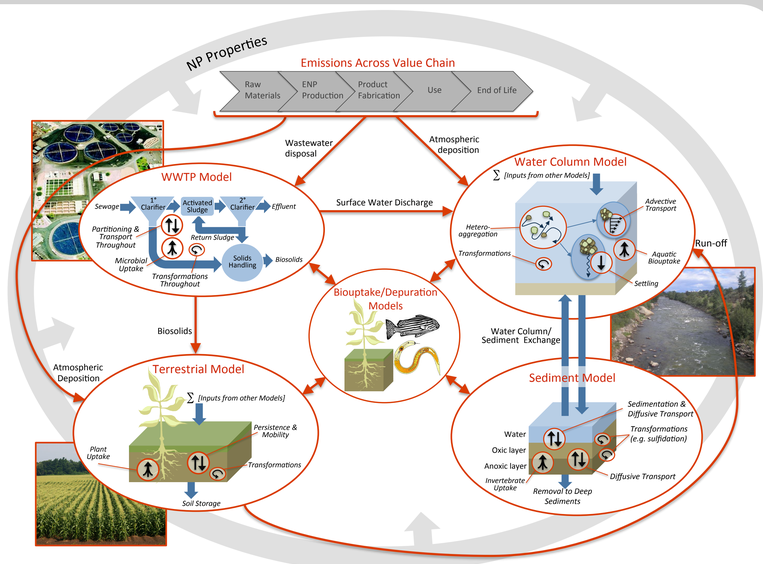
- The CEINT IKC is designed to support queries at a higher altitude to interrogate how Functional Assays can be used as a realistic categorization strategy for nanomaterials
- Functional Assay Parameters are aggregated, empirical measurements of NM behaviors in specific systems
- We query relationships between FA Parameters and
  1. Effects of interest, including ecological effects, toxicological effects, and possibly performance of ENMs.
  2. Core material and system properties, to ultimately work toward enabling QSAR approaches.



Framing Realistic Scenarios with Integrated Model Estimates

The CEINT IKC is designed to incorporate experimental data and model estimates of scenario parameters important for forecasting behavior and risks of nanomaterials.

- Estimated material release rates
- Estimated material transformation rates
- Estimated bioaccumulation rates and factors
- Estimated mobility and persistence



REFERENCES

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