Nanoparticle Surface Affinity as a Predictive Functional Assay

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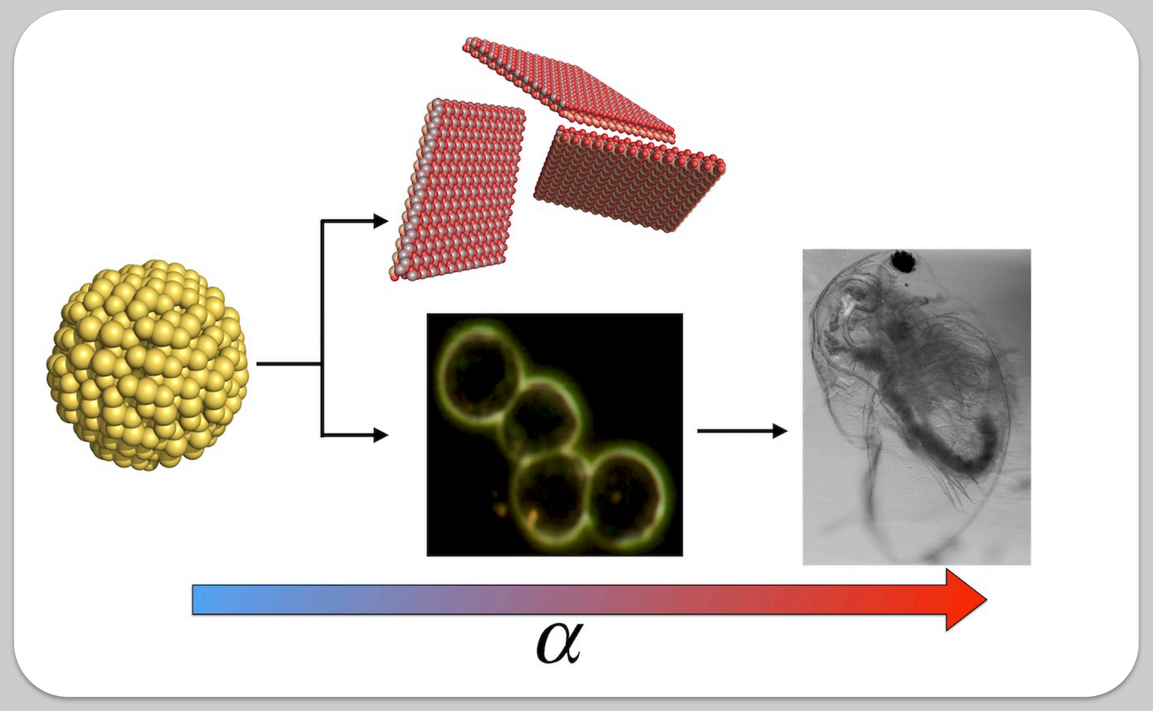
CEINT Center for the Environmental Implications of NanoTechnology

Functional assay design for nanoparticle surface attachment reflects the dual aspects of the CEINT Mission:

- To elucidate general principles that determine nanomaterial behavior in the environment → ***Functional assays 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. → ***Functional assays must support near-term risk-based decisions***

Surface Affinity Functional Assay Objectives

- Develop a benchtop functional assay for determining the efficiency of nanoparticle surface attachment, "alpha", on representative environmental surfaces
  - Should be simple to perform, flexible to various exposure scenarios, and applicable to the broadest range of nanomaterials possible
- Determine what factors drive differences in surface attachment efficiency, thereby increasing its predictive power
  - Examine various classes of nanoparticle surface chemistries, varying parameters such as surface charge, hydrophobicity, and stability
  - Utilize an array of attachment surfaces, including model glass beads, natural clays, soils, and biological matter
- Design consistent, relevant systems of materials and media, factoring in:
  - Nanoparticle of interest
  - Select a surface to which it will attach in the functional assay to closely mimic the environmental exposure scenario
  - Control and measure environmental parameters such as realistic solvent, pH, ionic strength and composition
- Evaluate and develop models to harness the predictive capacity of the functional assay
  - Develop a mathematical model for how surface attachment efficiency (α) might predict complex phenomena such as trophic transfer
  - Experimentally verify the link between trophic transfer and α
  - Expand predictive models to other systems, including watershed transport, soil system transport, and plant uptake potential



REFERENCES

This Poster

The work in this poster is presented in more detail in the following publications:

Geitner, N. K.; Marinakos, S. M.; Guo, C.; O'Brien, N.; Wiesner, M. R., Nanoparticle Surface Affinity as a Predictor of Trophic Transfer. Environmental Science & Technology 2016, 50 (13), 6663-6669.

Hendren, C. O.; Lowry, G. V.; Unrine, J. M.; Wiesner, M. R., A functional assay-based strategy for nanomaterial risk forecasting. Science of The Total Environment 2015, 536, 1029-1037.

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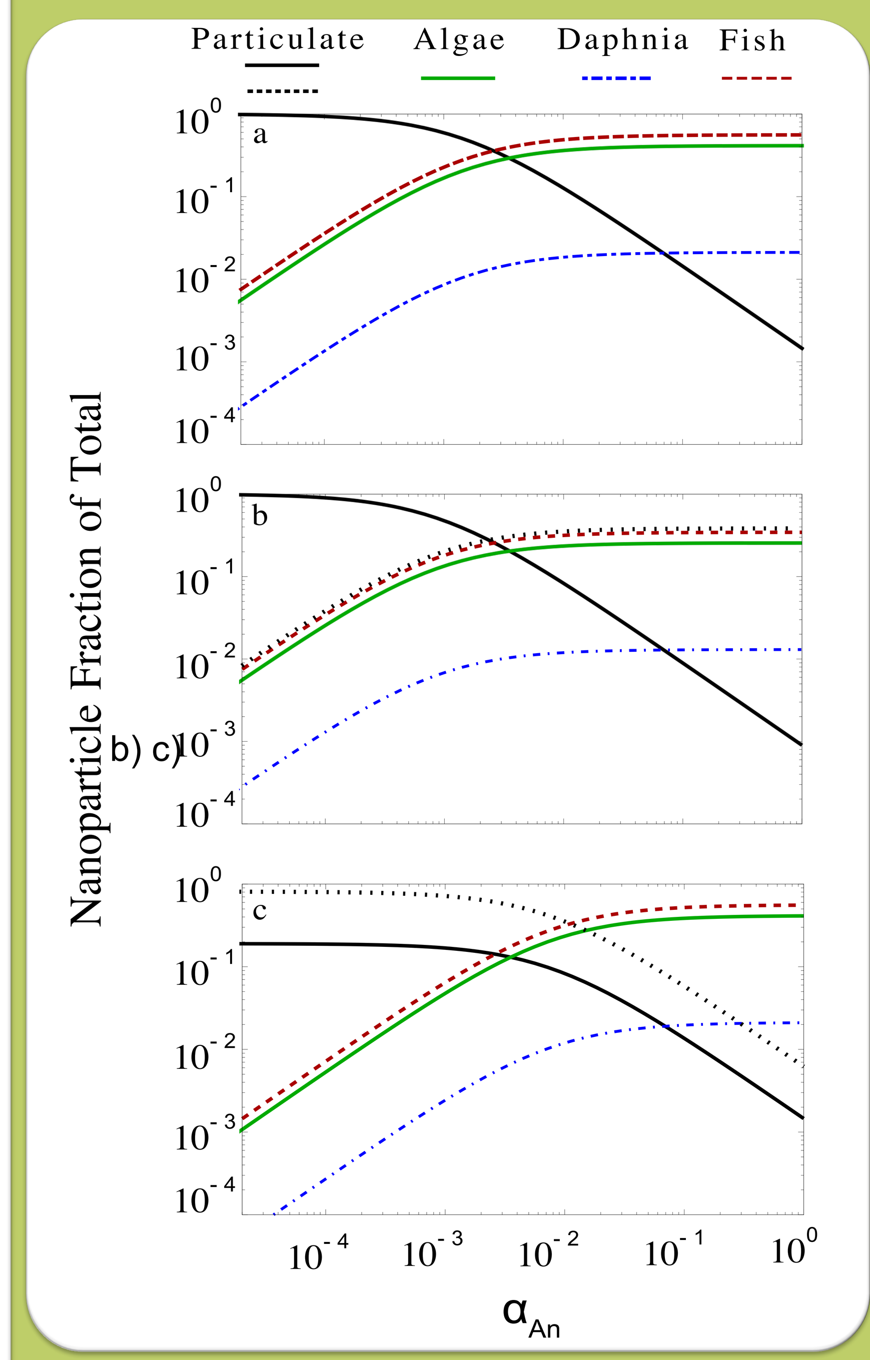
Model for Predicting Trophic Transfer from Surface Affinity (α)

The calculated relative fractions of nanoparticles present in different environmental compartments, including particulate (free or attached to colloids), live algae, daphnia, and fish representing a small, model ecosystem.

The three panels below represent different environmental scenario assumptions.



a) In this scenario, there are no background colloids (i.e. Clays, etc), and so no competitive adsorption of nanoparticles onto these surfaces.

b) In this scenario,, there are clays included in the model, and we assumed that attachment efficiencies onto these surfaces were equal to that on algae and other organisms.

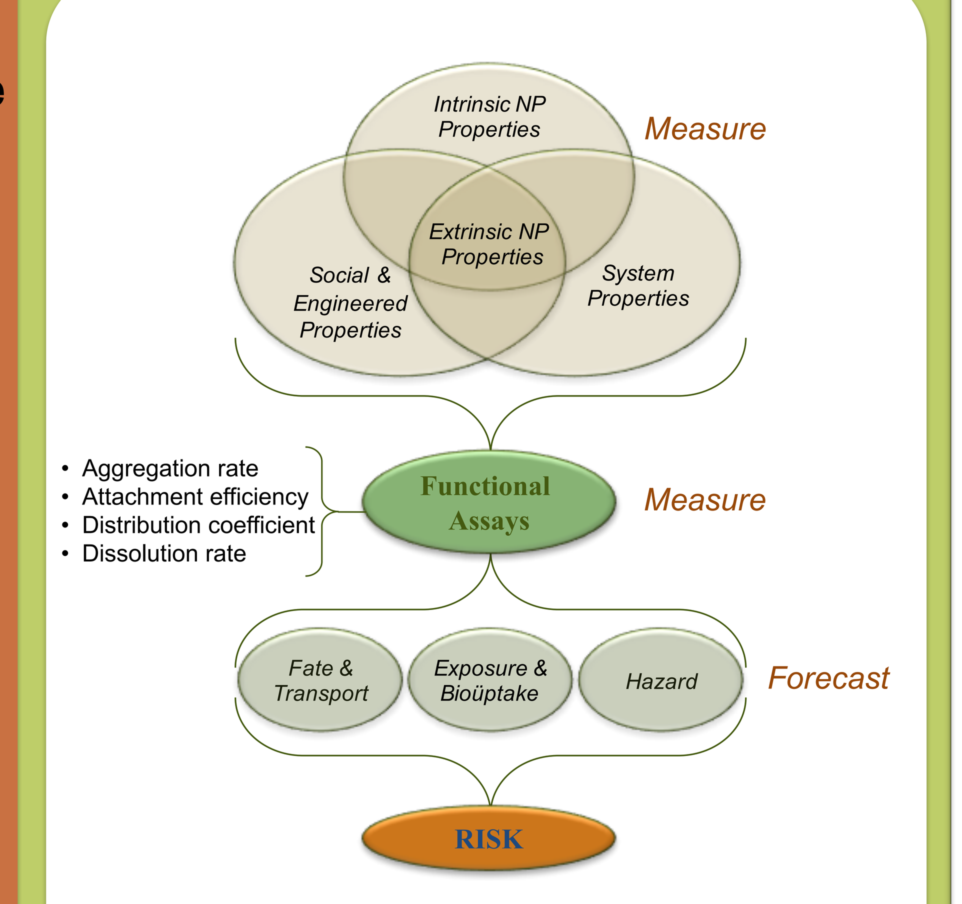
c) The scenario used the same concentrations of clay as in panel (b), but we assume that attachment efficiency of nanoparticles onto clay is independent of that onto biological surfaces.

A higher alpha leads first to more attachment of nanoparticles to the base of the food chain, and subsequently directly leads to greater trophic transfer.

Therefore α seems to be a strong and direct predictor of trophic transfer from just this simple functional assay.

Functional Assay Testing for Forecasting ENM Behavior, Performance, and Impacts

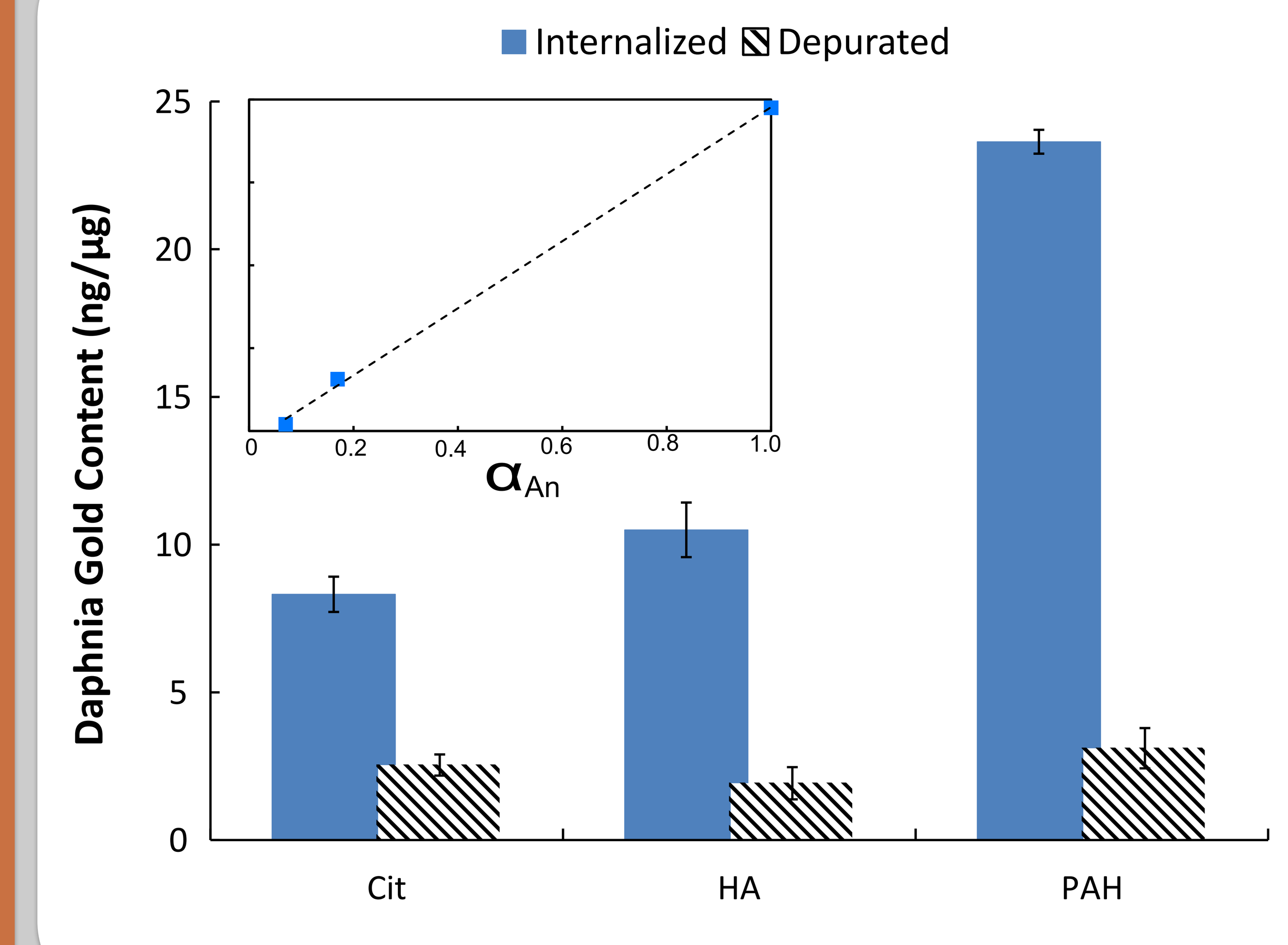
- Approaches to predict behavior and risk directly from nanomaterial (NM) properties are problematic
- We propose functional assays (FA) to measure nanomaterial behavior in systems
- FAs produce intermediary, empirical measurements of NM behaviors in specific systems, providing parameters parameters that bridge the gap between nanomaterial properties and potential outcomes
- FAs measure NM processes in prescribed systems to parameterize exposure, hazard models
- FAs can support near-term nanoEHS guidance, mechanistic research based on upstream properties, and sustainable product development



A Simple Assay for Powerful Predictions

This graph shows the experimentally measured concentrations of gold found within daphnia after being fed algae that had been pre-exposed to gold nanoparticles of three different surface functionalities.

The direct correlation with alpha (inset) suggests that surface attachment efficiency of nanoparticles onto the surface of algae is highly predictive of this sort of trophic transfer.



Acknowledgements

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