Progress in modeling nanomaterial exposure

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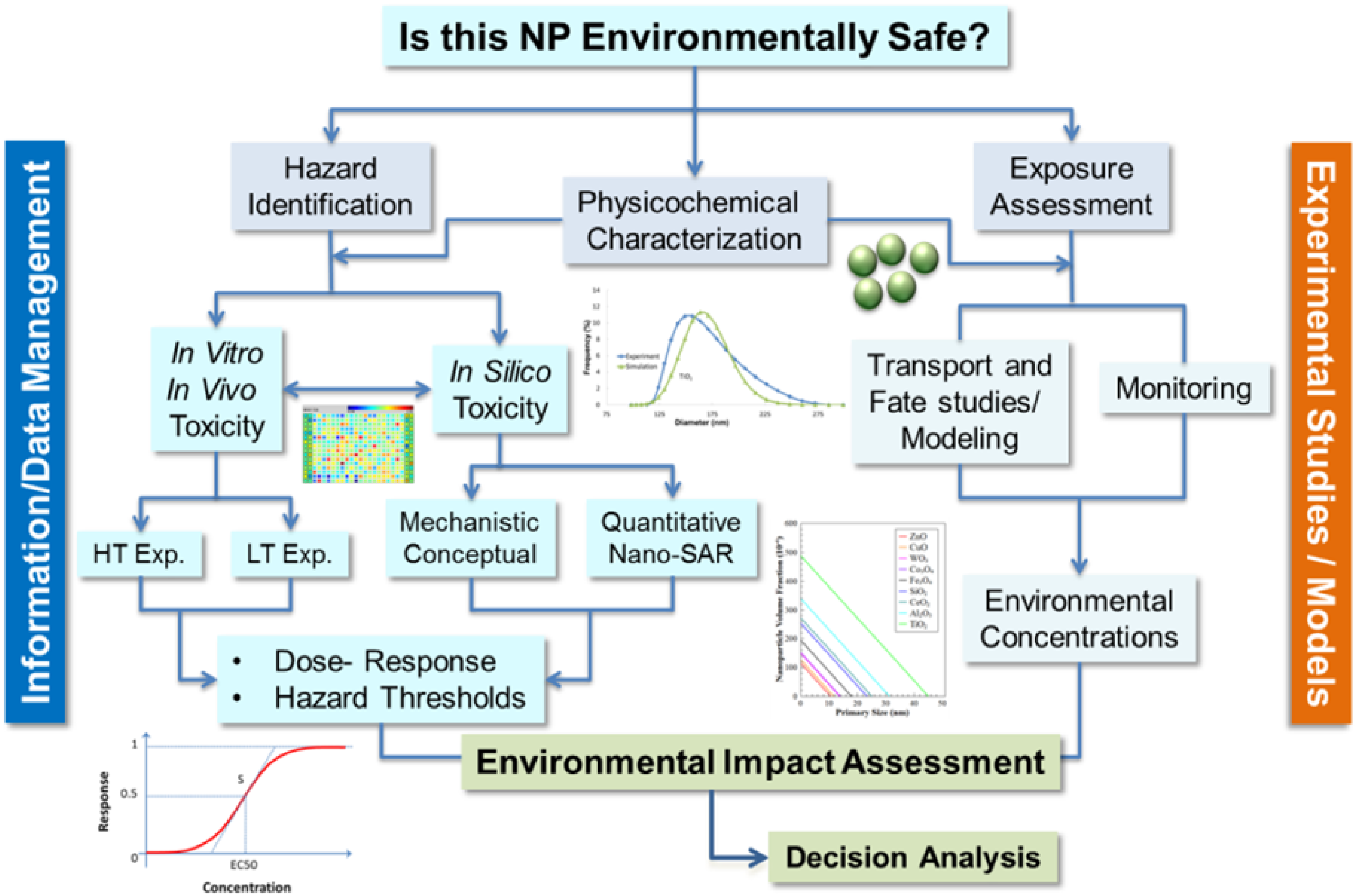
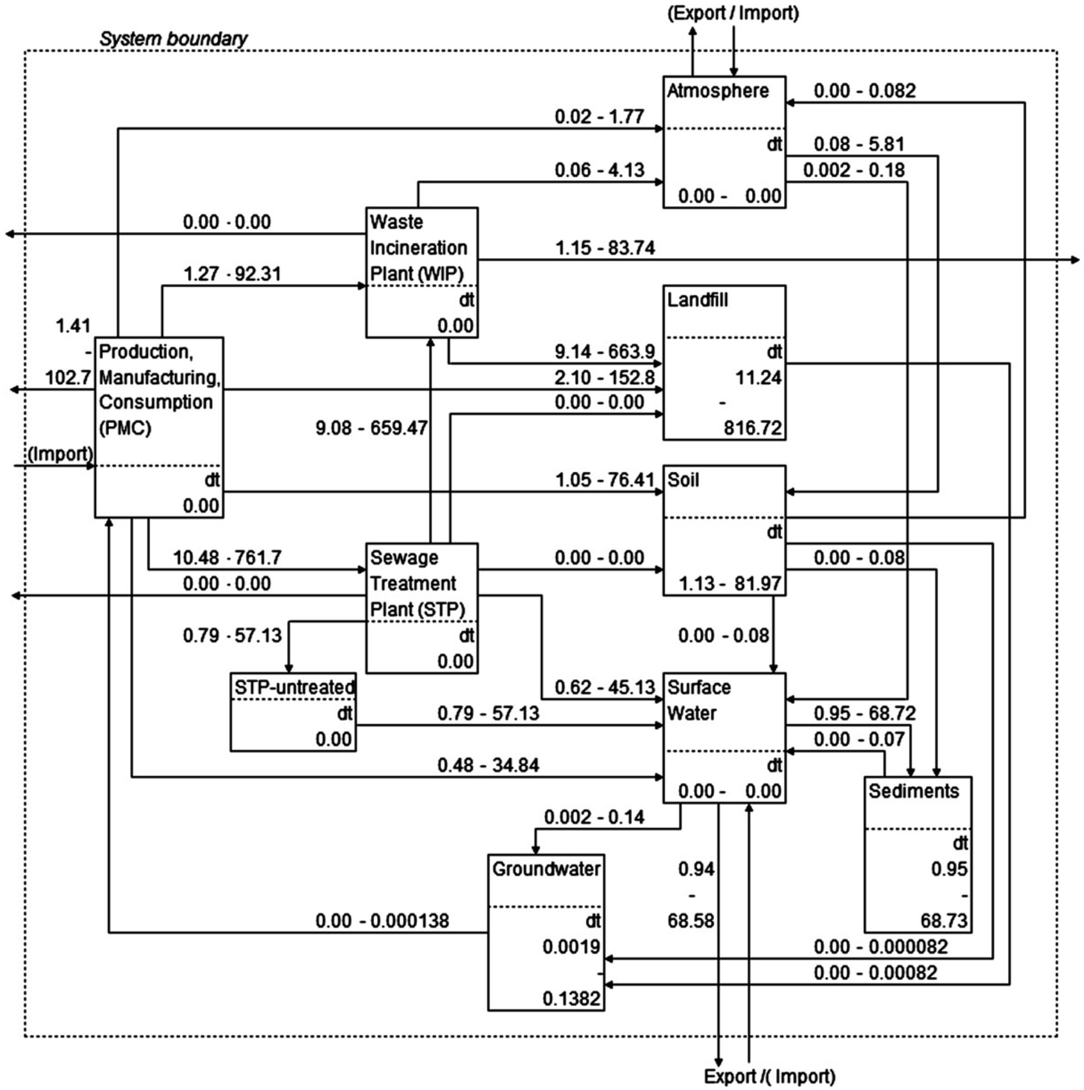


Yoram Cohen and co-workers, 2013

Probabilistic material flow modeling for assessing the environmental exposure to compounds: Methodology and an application to engineered nano-TiO_2 particles

Fadri Gottschalk [a,b], Roland W. Scholz [a], Bernd Nowack [b,*]

Environmental Modelling & Software 25 (2010) 320–332



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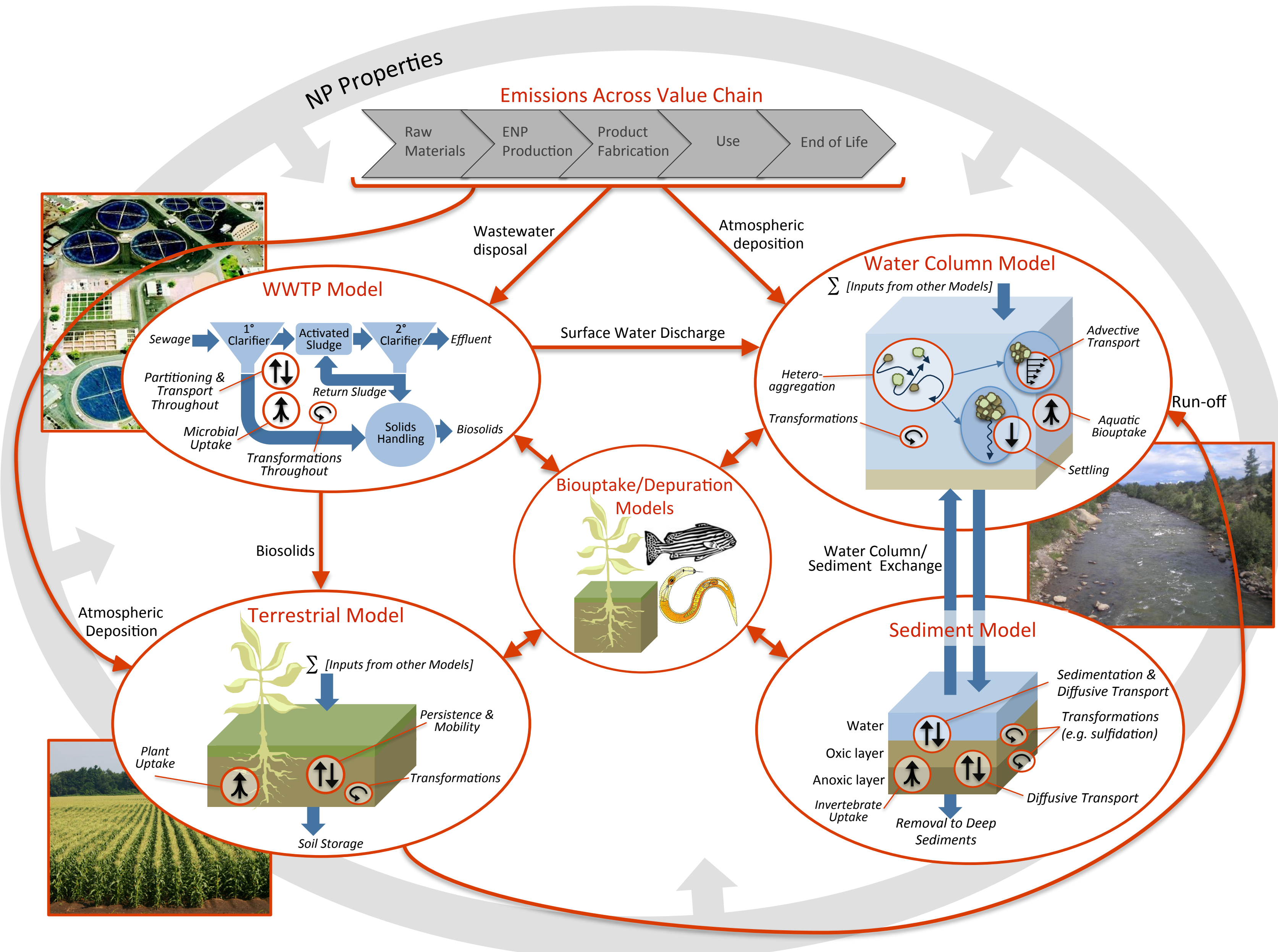

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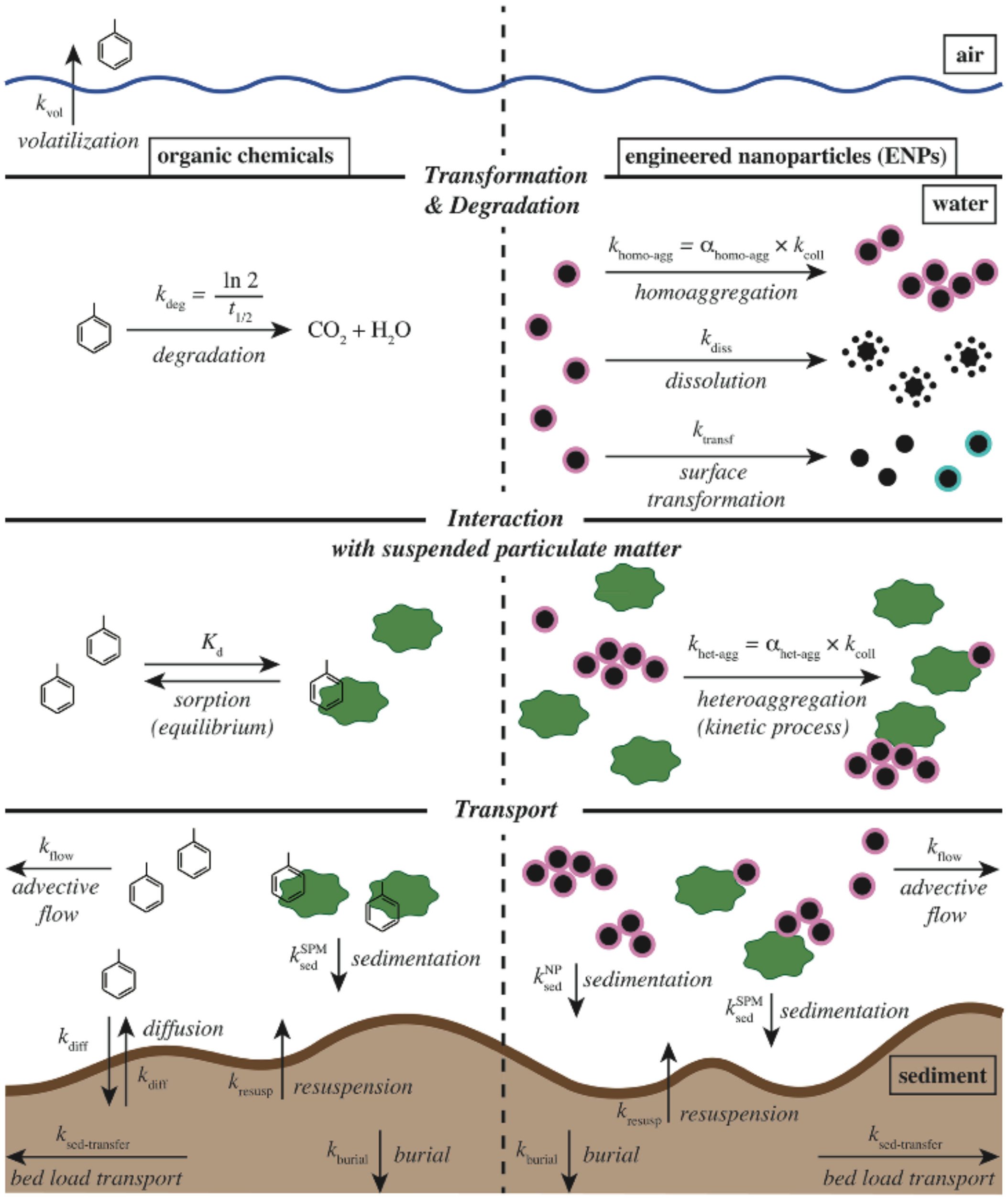
Praetorius, Scheringer, and Hungerbühler, 2012



Environmental Science & Technology

Article

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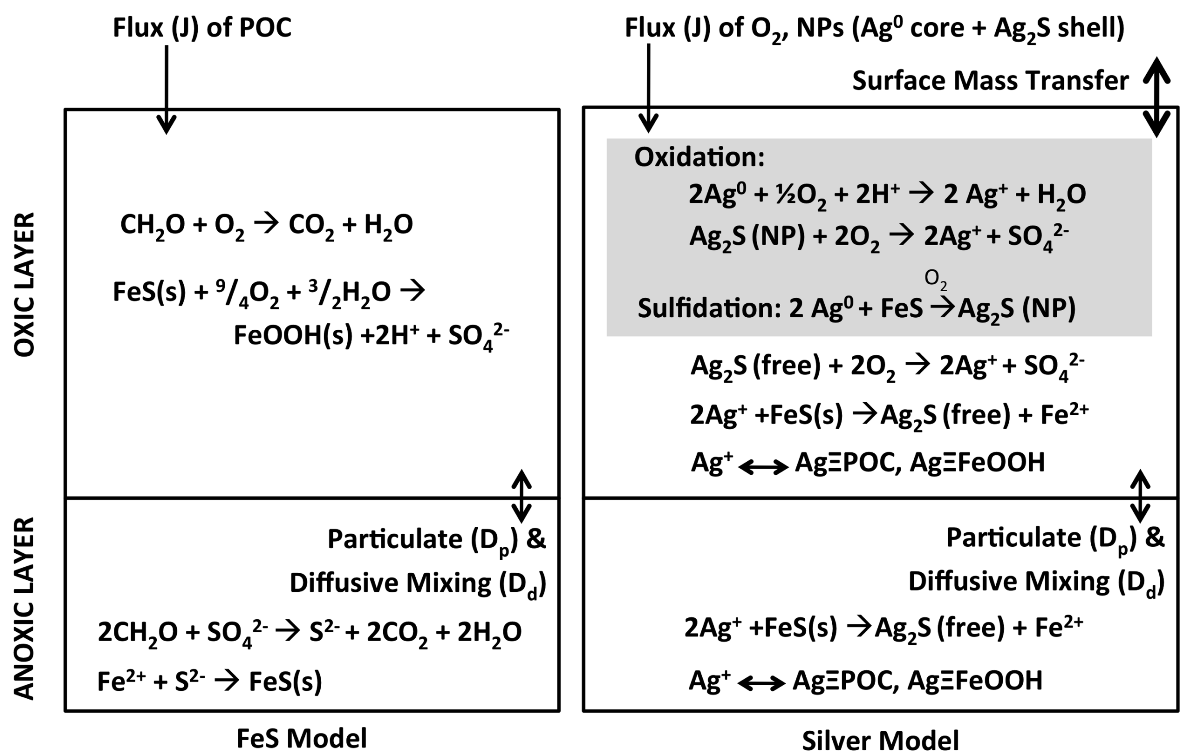
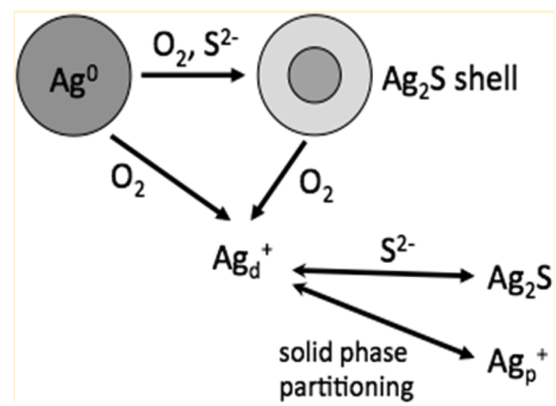
Modeling Nanosilver Transformations in Freshwater Sediments

Amy L. Dale,[†,‡] Gregory V. Lowry,[†,§] and Elizabeth A. Casman[†,‡,*]





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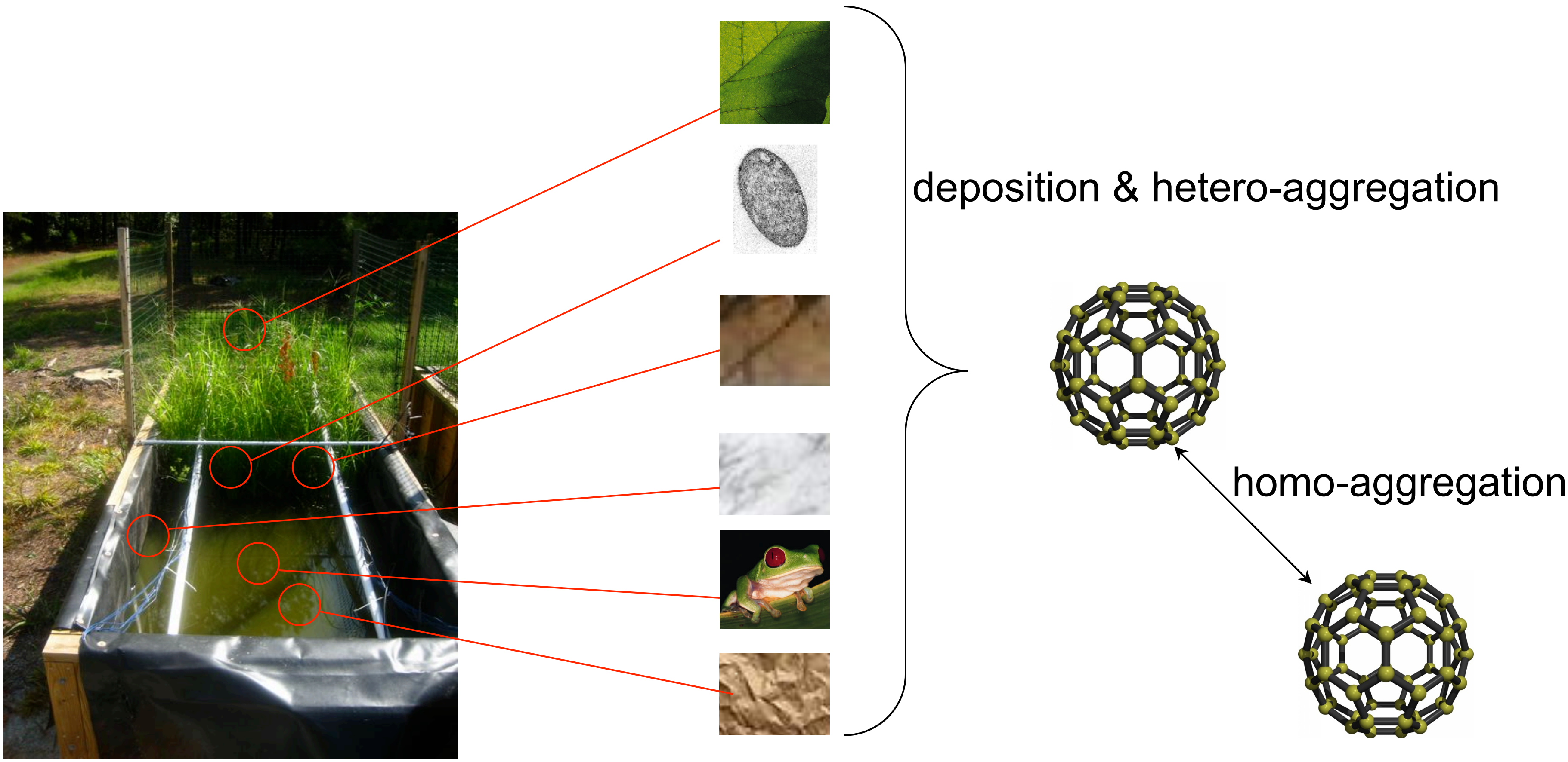
Affinity of nanoparticles for various surfaces



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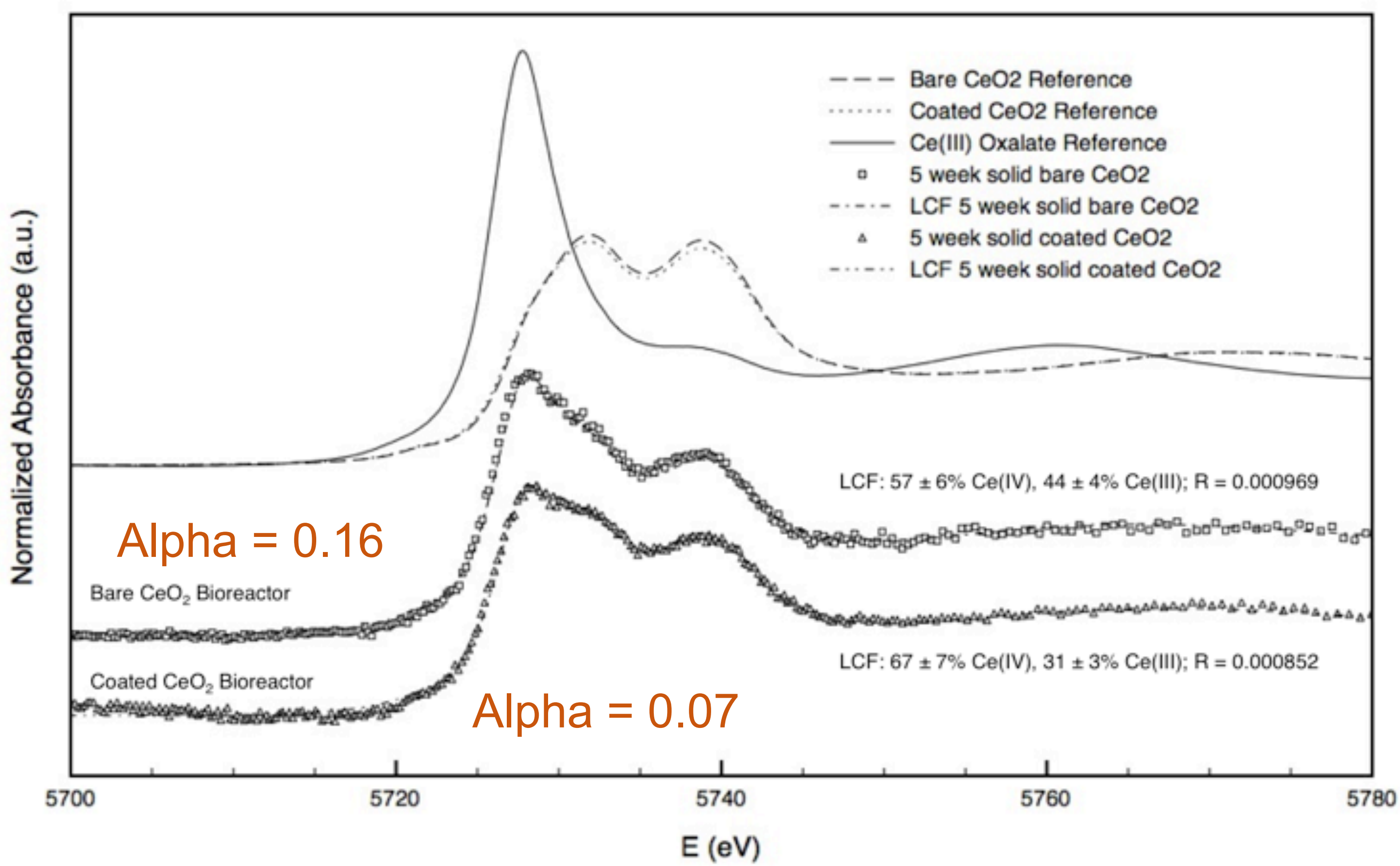
Importance of surface affinity for transformtion: CeO2



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Lauren Barton (Duke University & CEREGE, France)

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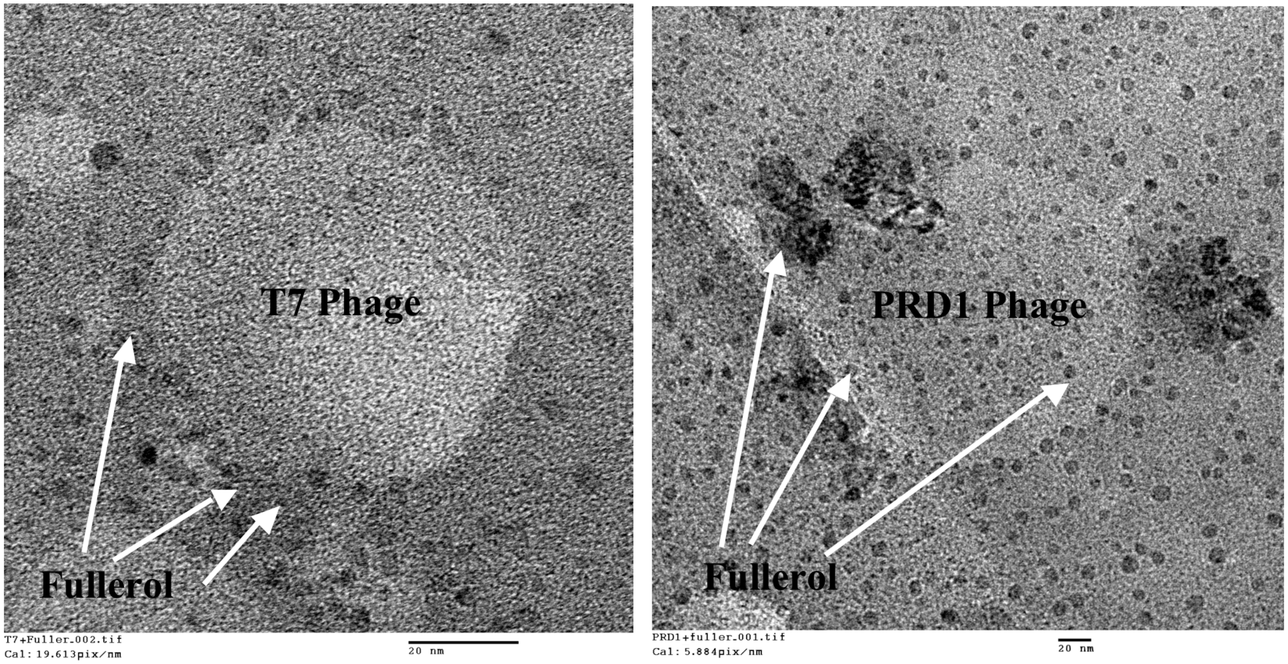

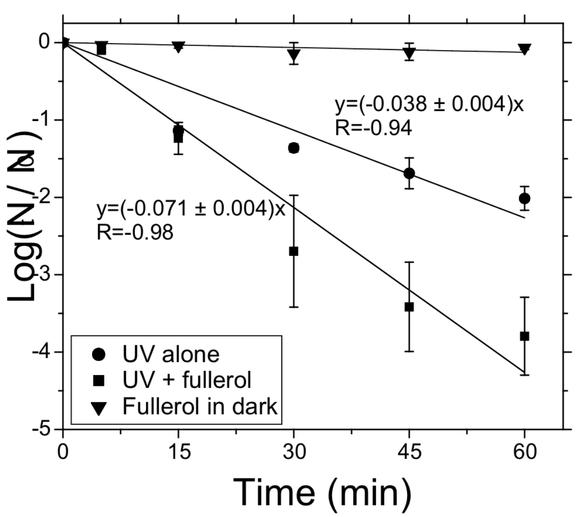

Raju Badireddy, Duke University

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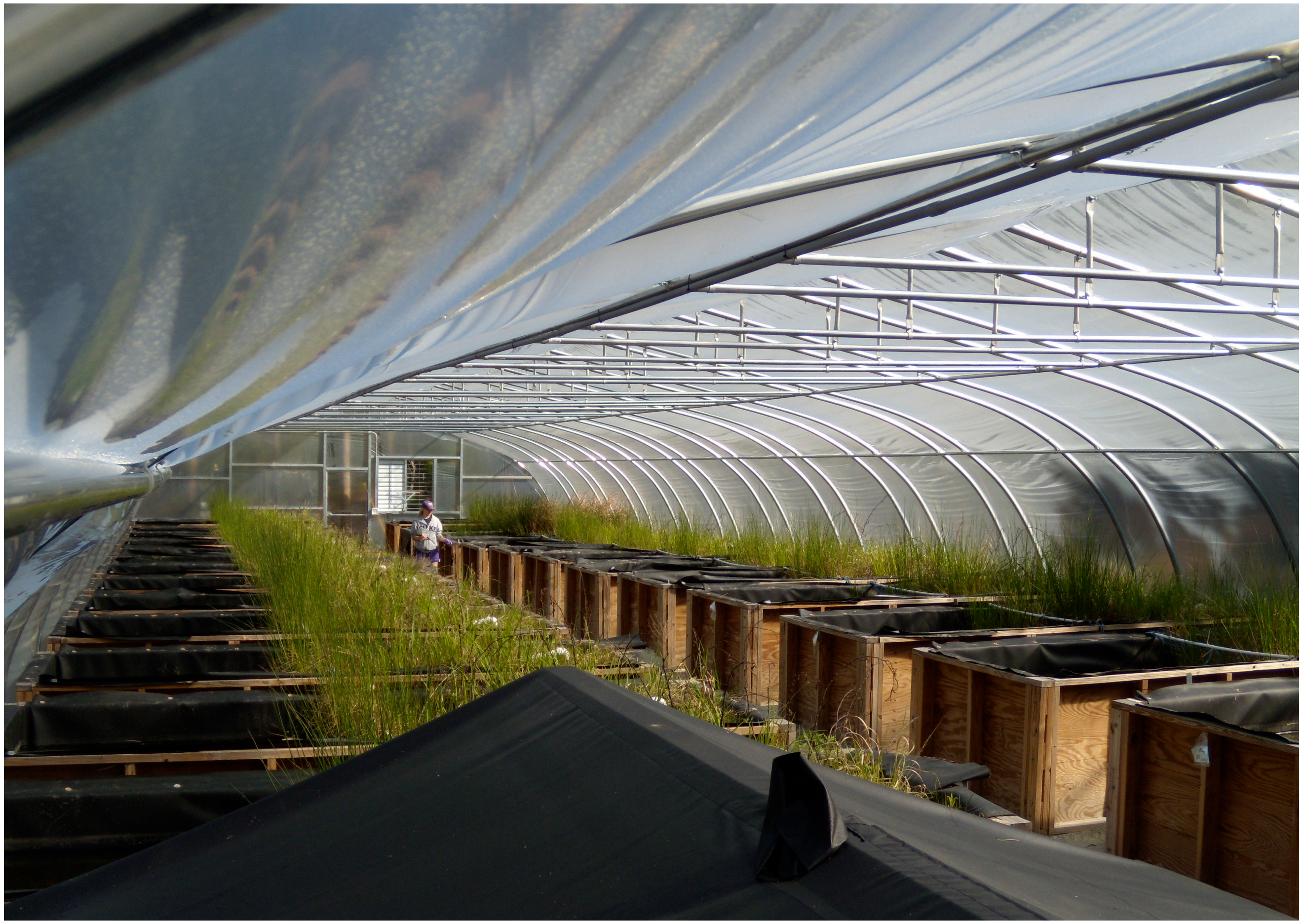
Mesocosms:
Controlled Release Field Sites



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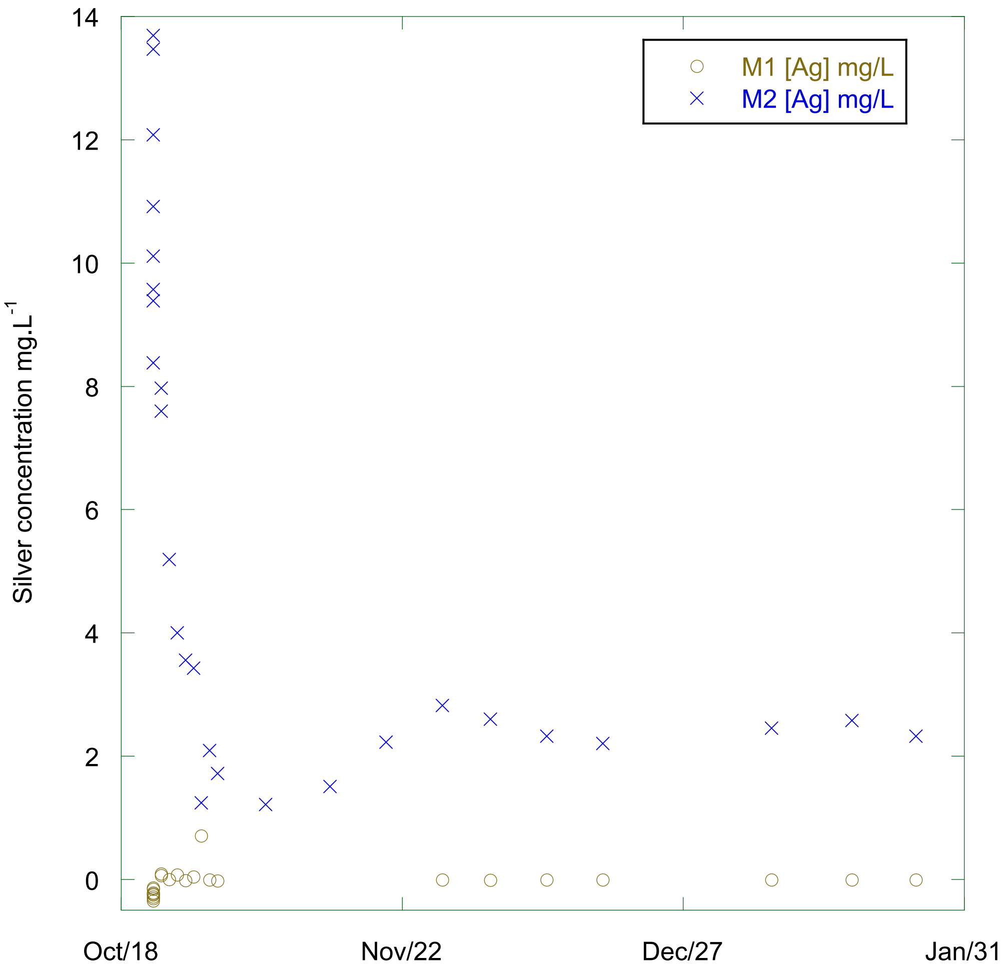
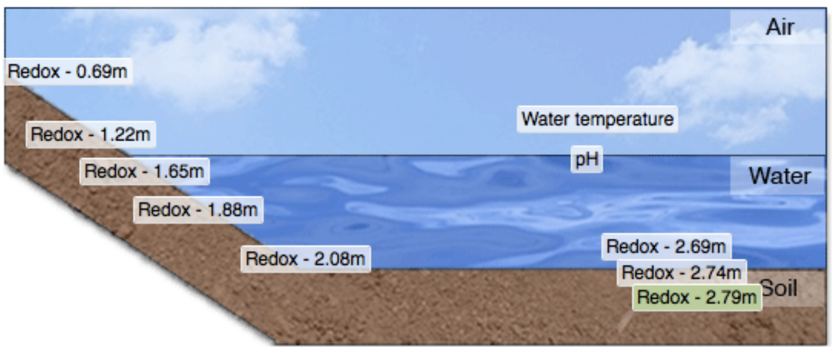
Nanosilver removal in CEINT mesocosms





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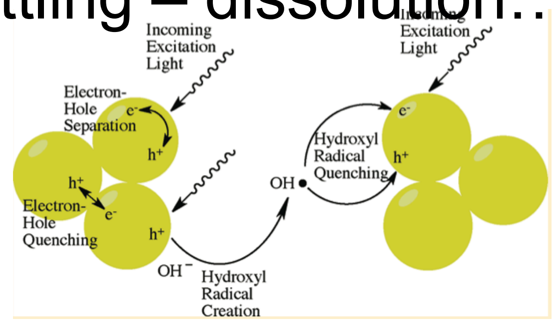
Aggregation, Transport and Surface affinity

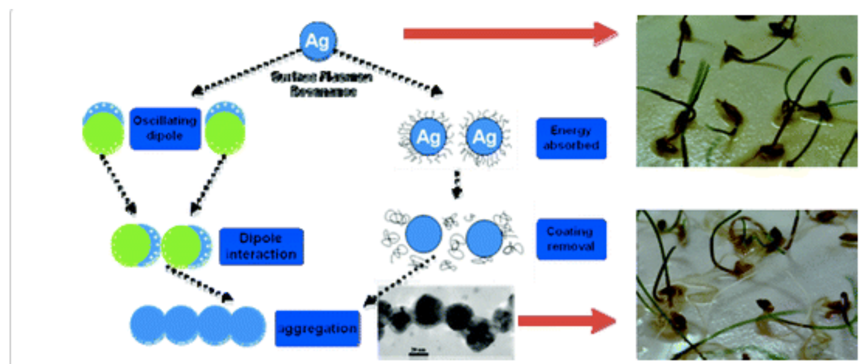
$$\frac{dn_k}{dt} = \frac{1}{2}\sum_{i+j=k} \alpha\left(f_i,f_j\right)\beta\left(r_i,r_j,f_i,f_j\right)n_i n_j - n_k\sum_{i} \alpha\left(f_k,f_i\right)\beta\left(r_k,r_i,f_k,f_i\right)n_i$$

+/- breakup –settling – dissolution…

Aggregation:
- *Dissolution*
- *Reactivity*
  - *Photo-catalysis*
  - *Molecular Adsorption*
- *transport*

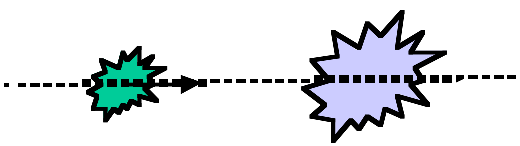
Deposition:
- *Environmental dispersal*
- *Biouptake*
- *Translocation in organisms*





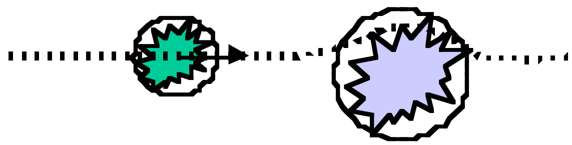
Modeling collision rate coefficients and drag coefficients on aggregates (transport)

Rectilinear Model



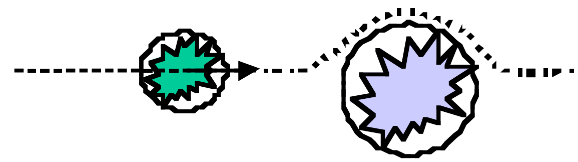
Smoluchowski, 1917

Intermediate model

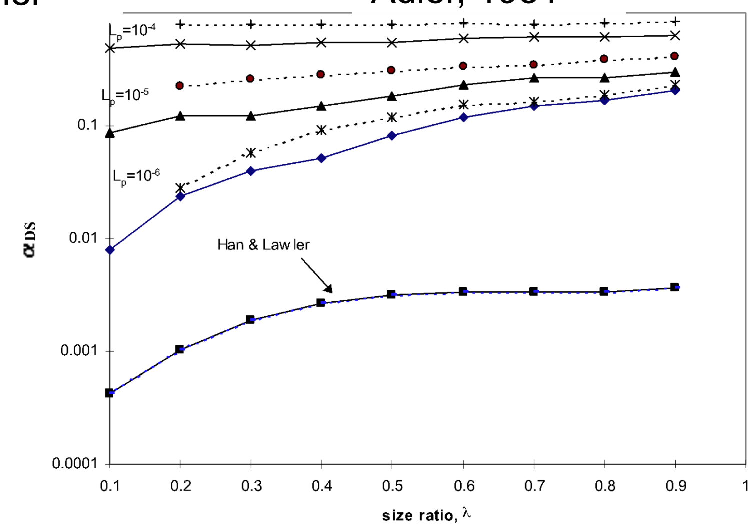


Veerapaneni and Wiesner 1997

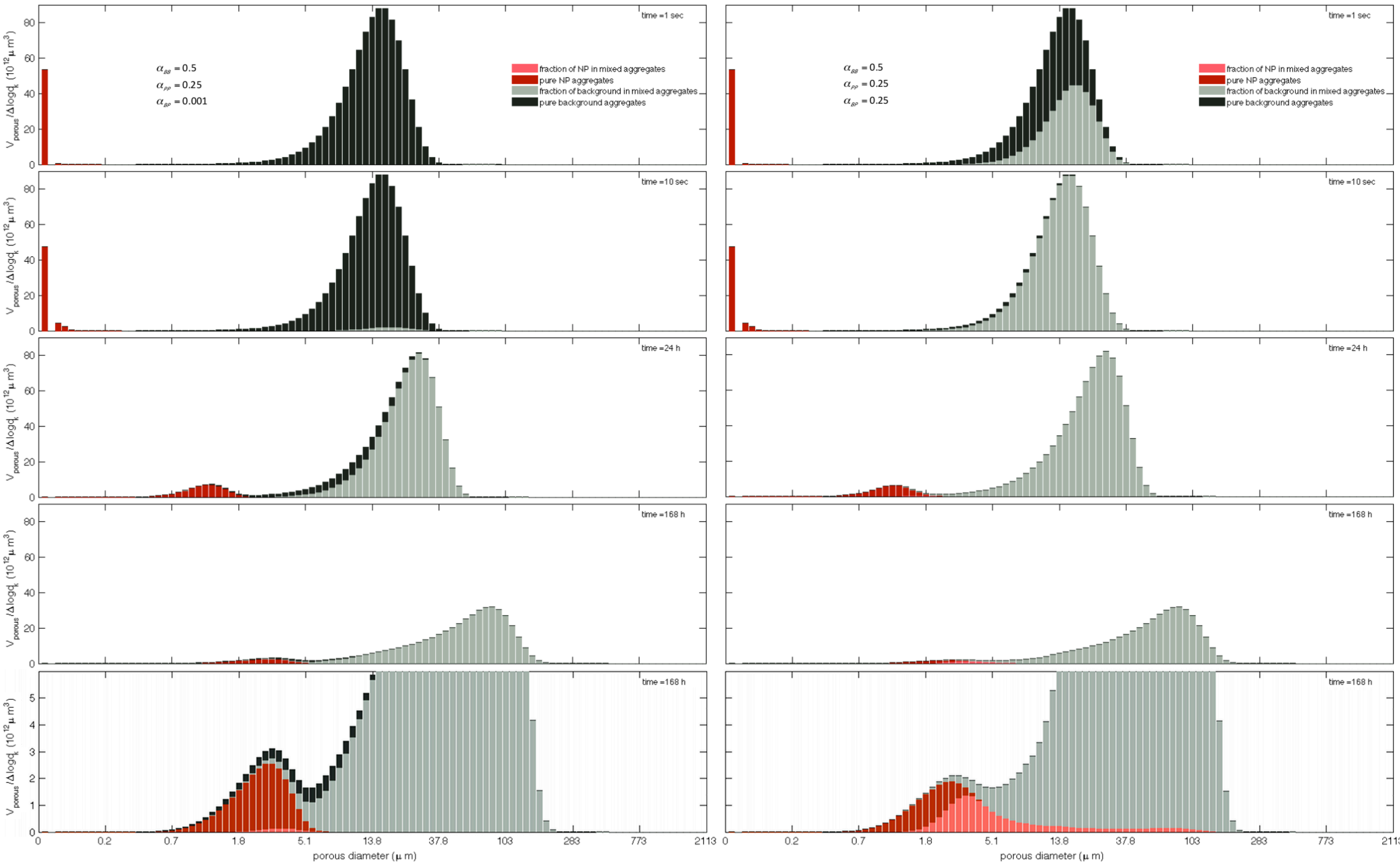
Curvilinear Model

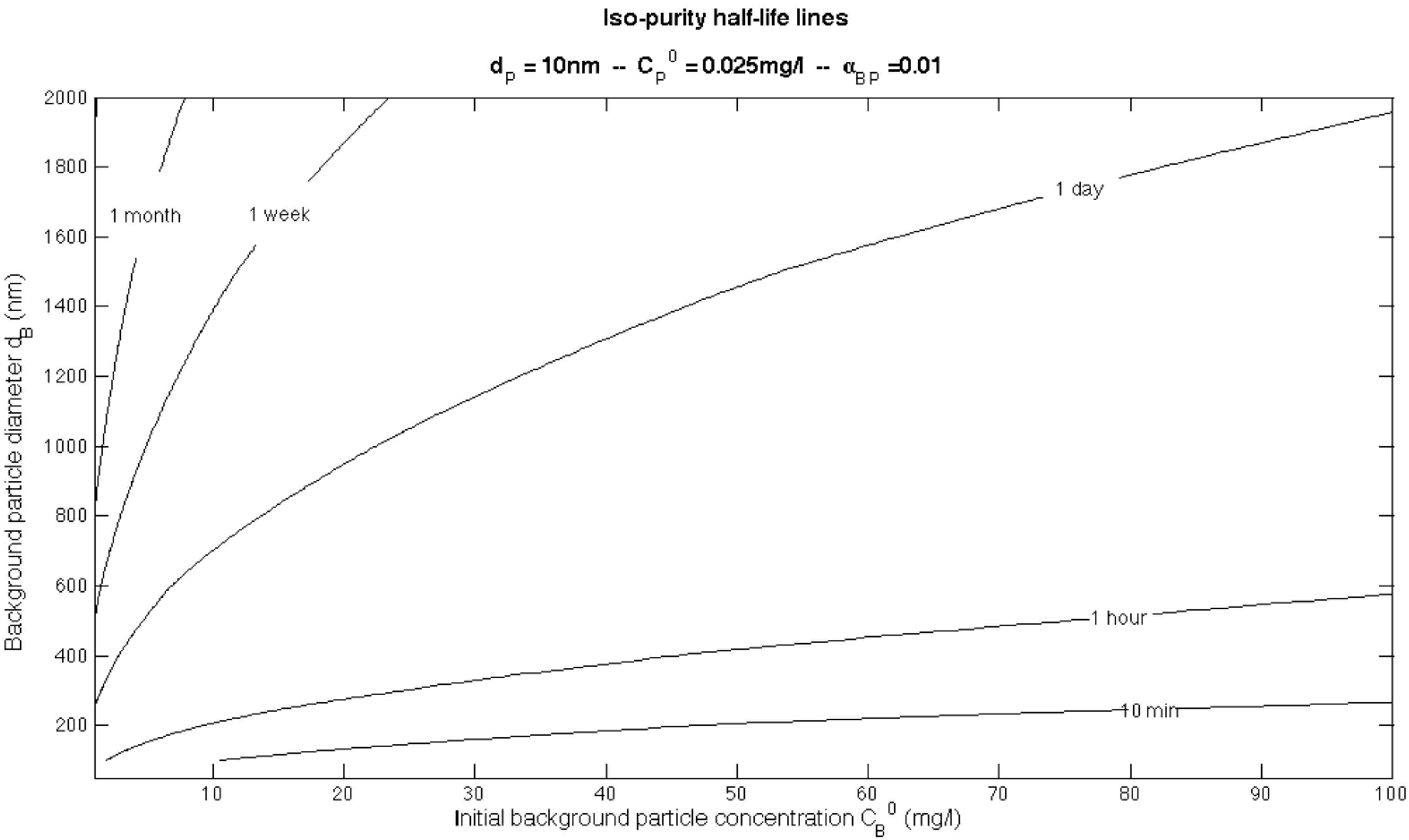


Adler, 1981

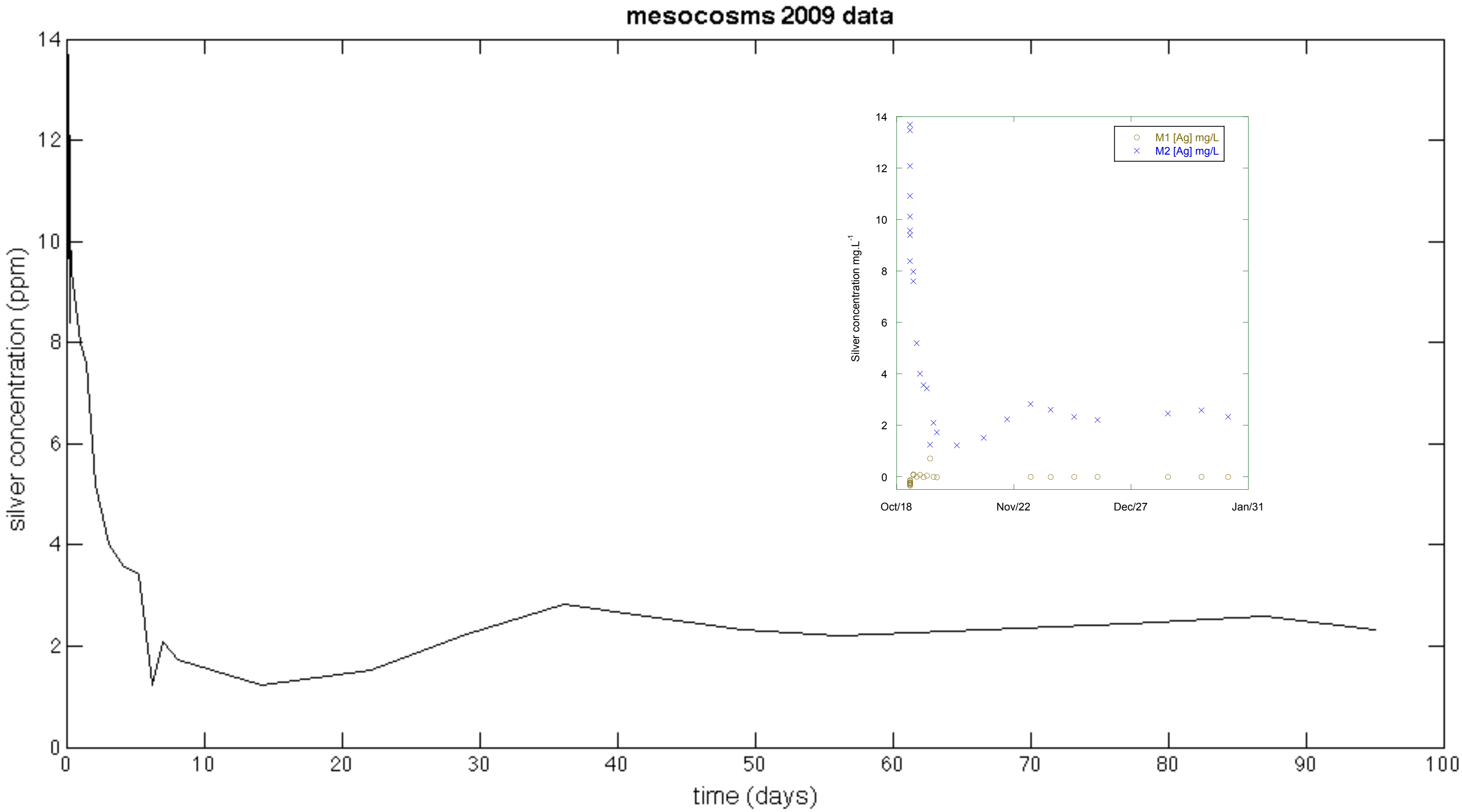


Simulations of heteroaggregation





Iso-purity half-life lines
d_p = 10nm -- C_p^0 = 0.025mg/l -- α_{BP} = 0.01
1 month
1 week
1 day
1 hour
10 min
2000
1800
1600
1400
1200
1000
800
600
400
200
10
20
30
40
50
60
70
80
90
100
Background particle diameter d_B (nm)
Initial background particle concentration C_B^0 (mg/l)



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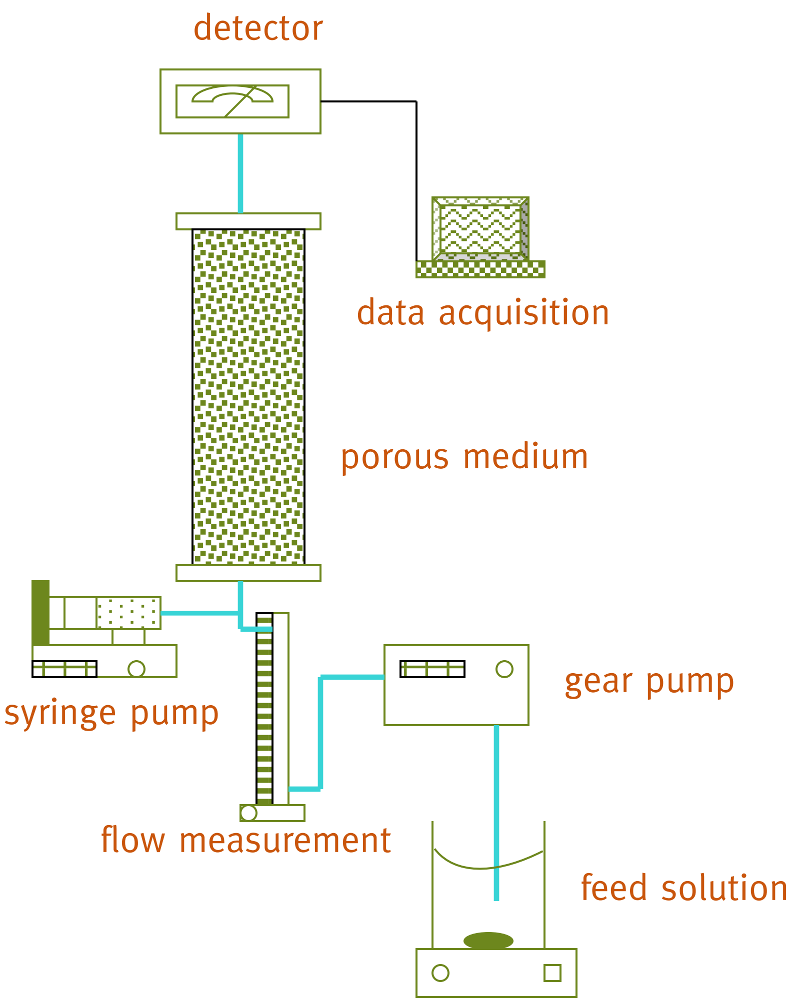
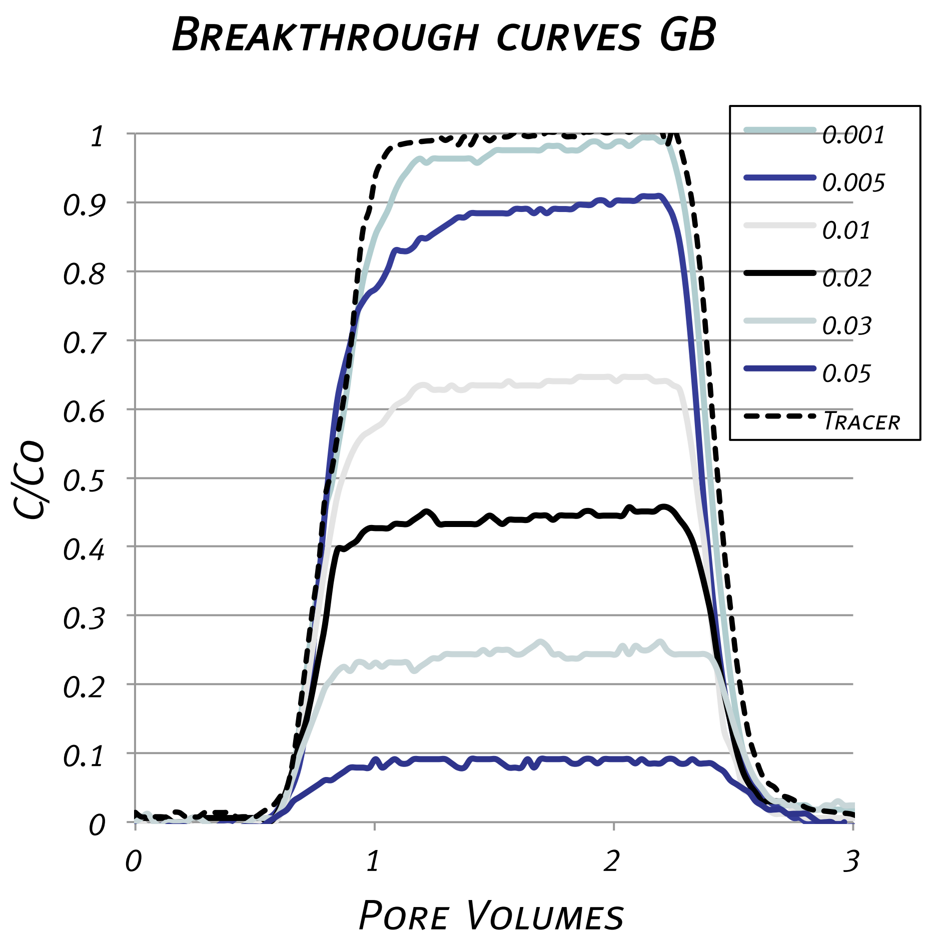
Measuring affinity (alpha) in model systems





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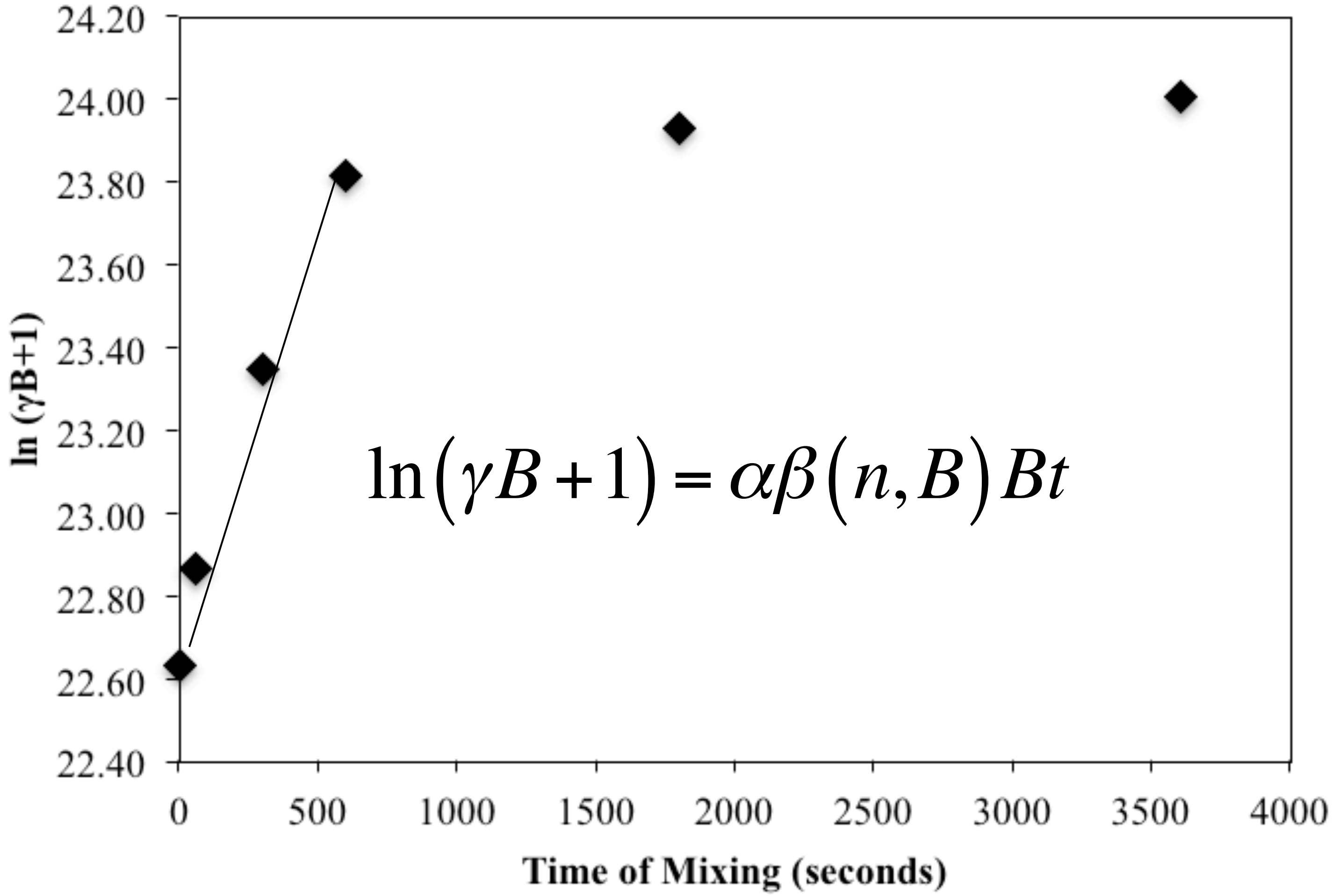
Measuring surface affinity in complex systems

$$\frac{dn_k}{dt} = \frac{1}{2}\alpha \sum_{i+j\to k} \beta(i,j) n_i n_j - \alpha n_k \sum_i \beta(i,k) n_i - breakup$$

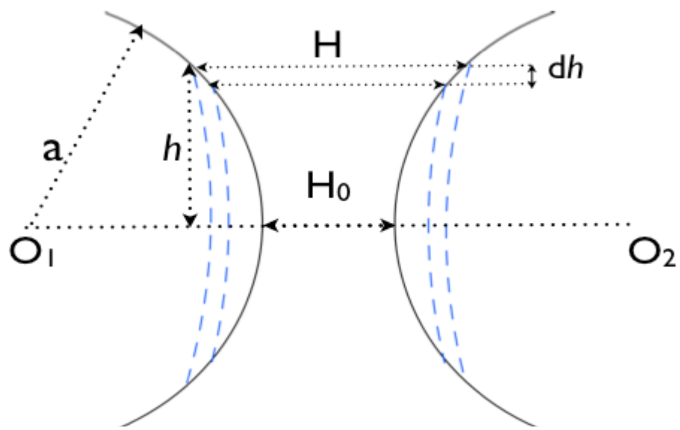
$$\frac{dn}{dt} = -\alpha\beta(n, B) nB + k_B (n_0 - n)$$

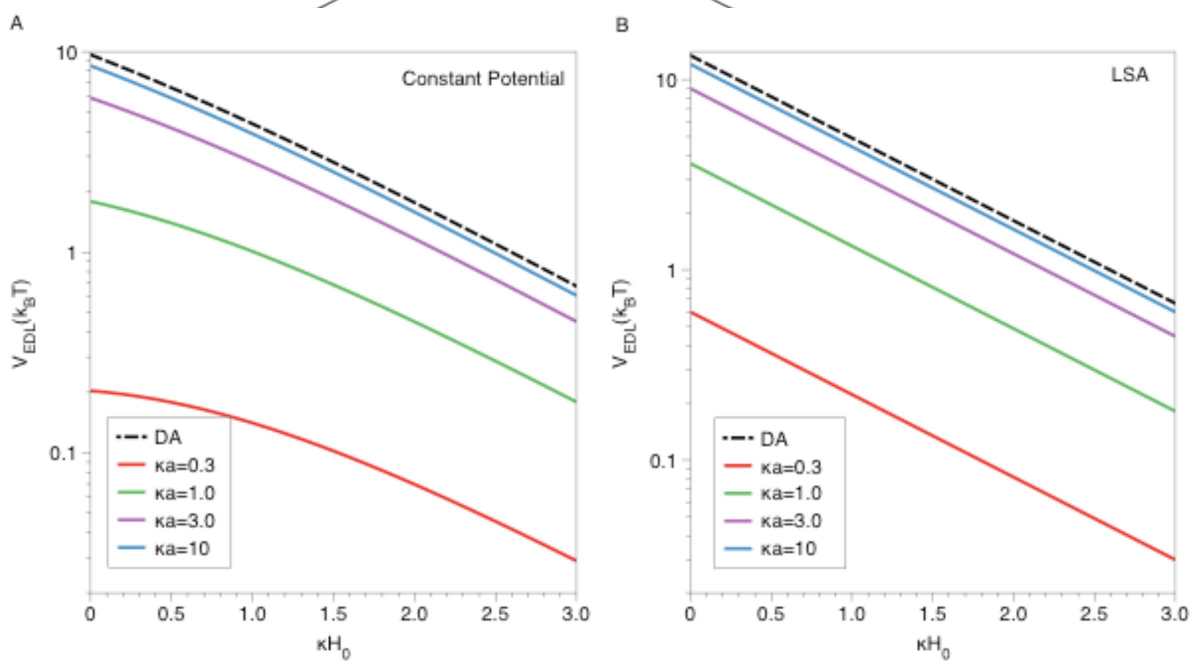
$$\alpha = \frac{\ln(\gamma B + 1)}{\beta B t} = \frac{\ln(\gamma B + 1)}{\beta B} * \frac{1}{t}$$

Transformed distribution coefficient aggregation time



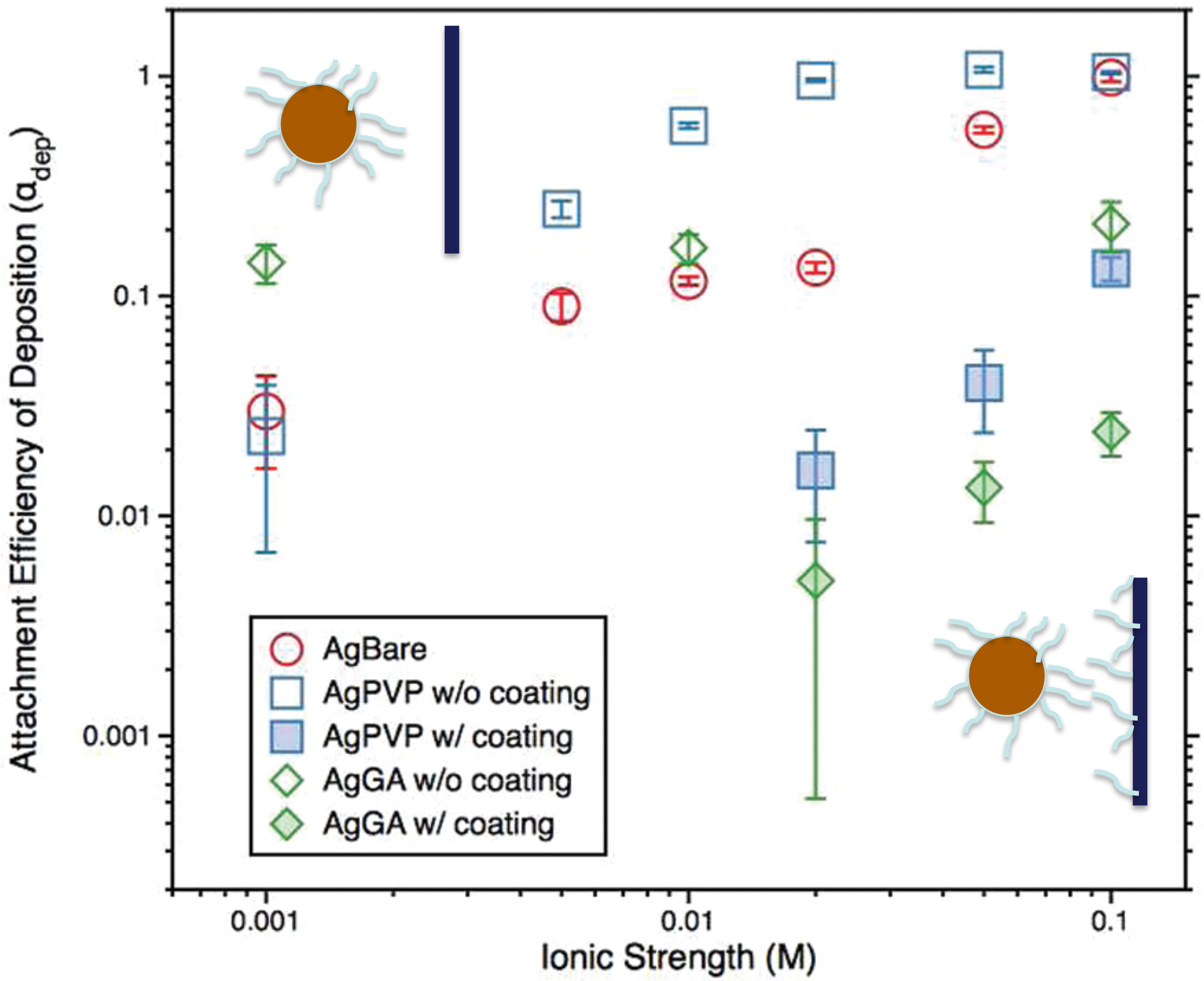
Predicting surface affinity from theory small κa and Derjaguin approximation





Energy of EDL interaction between a nanoparticle (a=10nm) and a flat plate based exact analytical expressions (A) constant potential; (B) linear superposition approximation

Asymmetry of surface coating may increase deposition



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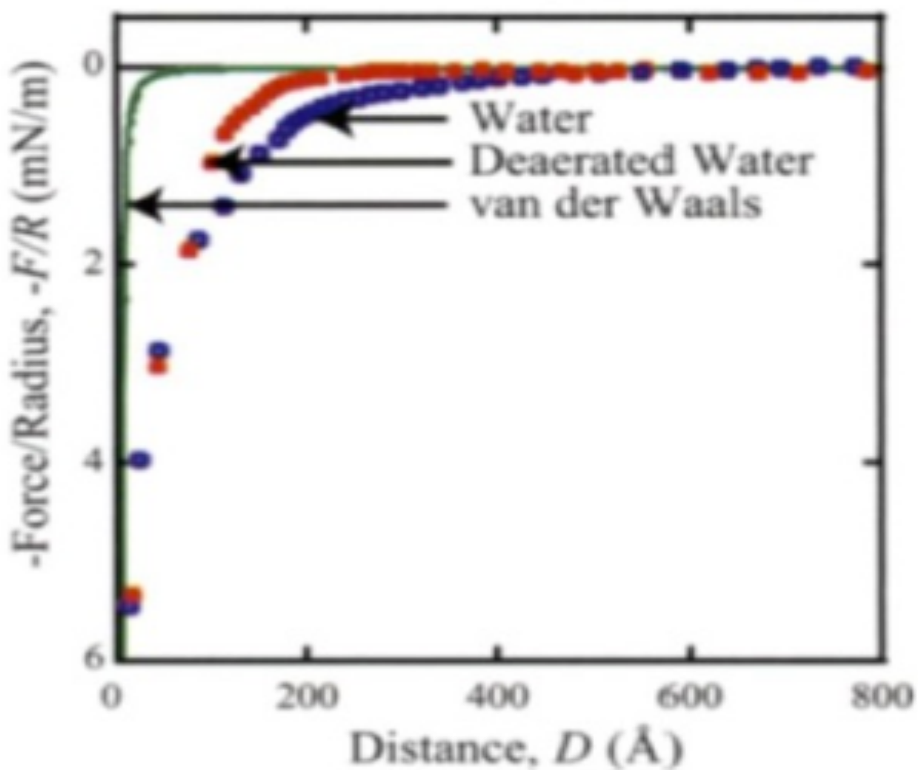
Hydrophobic interactions



Force - Separation distance profile between DODA-coated mica surfaces measured by dynamic surface force apparatus

Meyer, E. E.; Rosenberg, K. J.; Israelachvili, J., Recent Progress in Understanding Hydrophobic Interactions. *Proc. Natl. Acad. Sci.* **2006,** *103*, 15739-15746.

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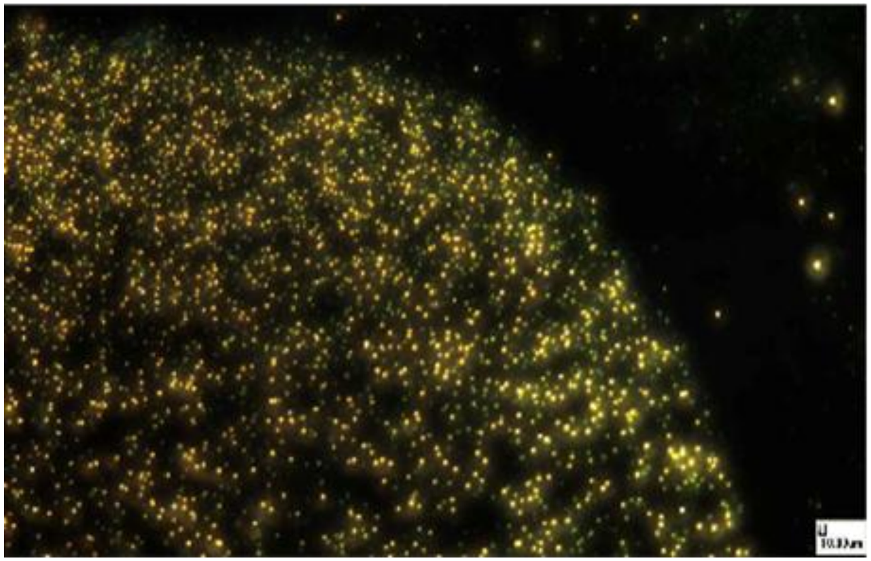
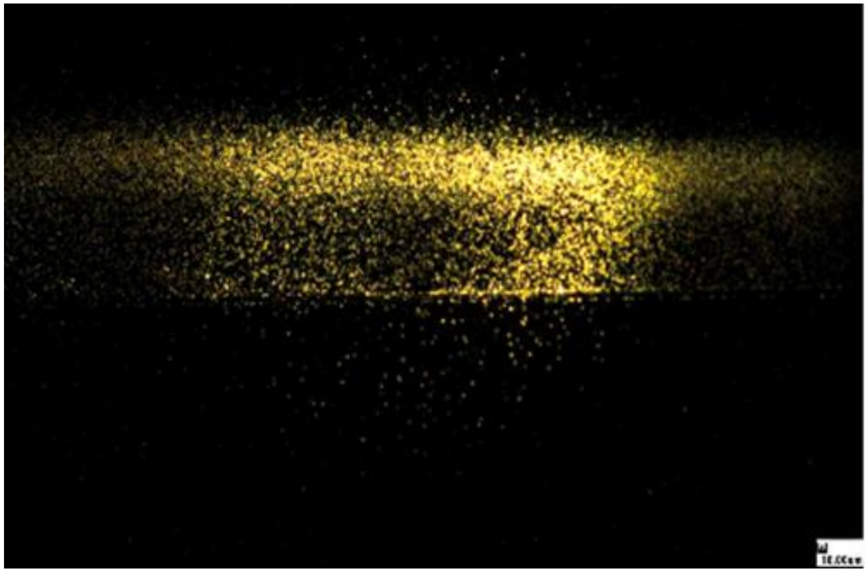
Possible methods for characterizing hydrophobicity

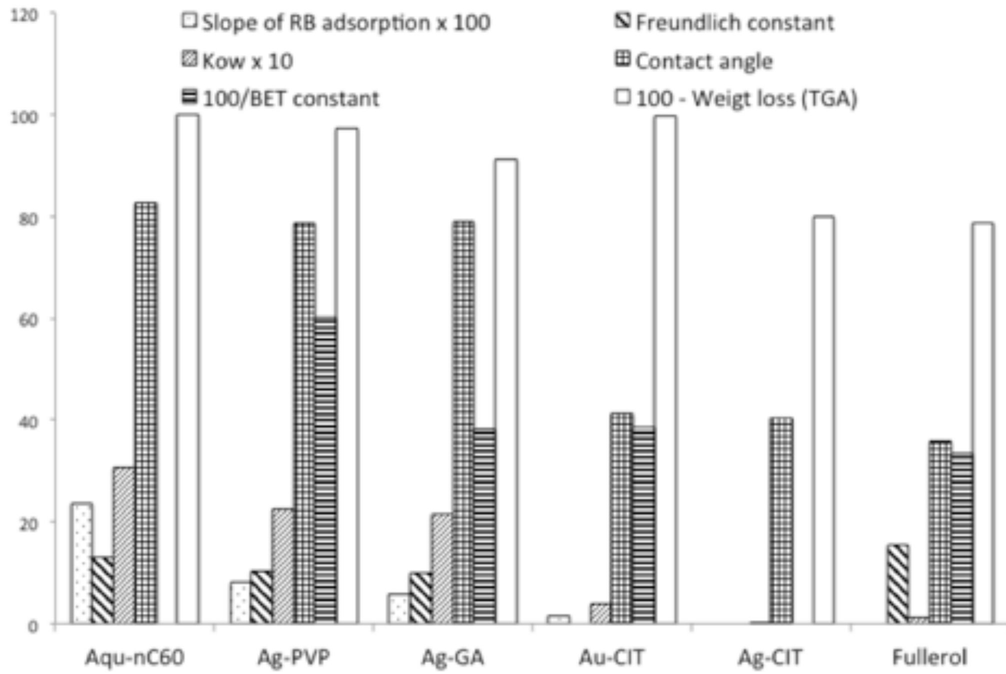
- K_{ow}
- Contact angle (lawn of nanoparticles)
- Adsorption of probe molecules
- Water adsorption
- Water desorption (TGA)

10 nm



100 nm





	AdsRB	AdsNPTL	K_{ow}	CA	cBET	TGA	immH	adsG
AdsRB	1	0.1691	0.905	0.85	-0.901	-0.8393	0.149	0.537
AdsNPTL	0.169	1	0.494	0.427	-0.394	0.0408	0.616	0.77
K_{ow}	0.905	0.4945	1	0.978	-0.838	-0.6698	0.231	0.642
CA	0.85	0.4274	0.978	1	-0.722	-0.6188	0.107	0.505
cBET	-0.901	-0.3943	-0.838	-0.722	1	0.6804	-0.292	-0.777
TGA	-0.839	0.0408	-0.67	-0.619	0.68	1	-0.374	-0.466
immH	0.149	0.6162	0.231	0.107	-0.292	-0.3743	1	0.74
adsG	0.537	0.77	0.642	0.505	-0.777	-0.4655	0.74	1

Concluding remarks

- *Need to connect exposure modeling and effects modeling*
- *Need to connect ambient concentration models to bioüptake models*
- *Need for functional assays to predict nanomaterial behavior*
- *Need for data on nanomaterial behavior in complex systems*
- *Need for data integration*

Acknowledgements

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United States Environmental Protection Agency

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