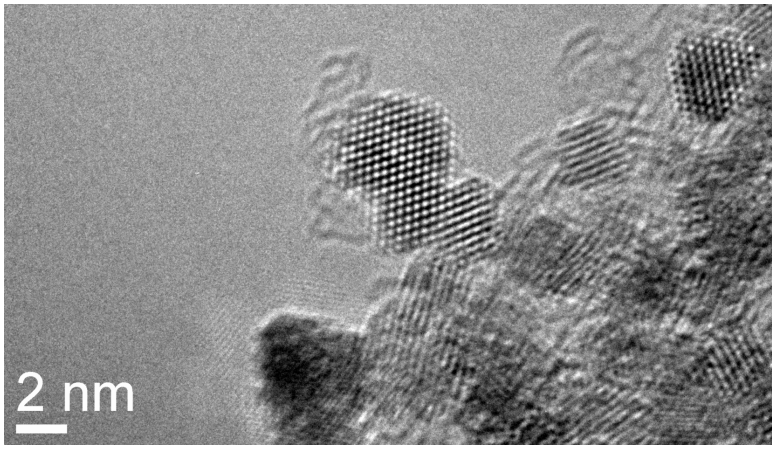
Nanoparticle coatings dominate their behavior in environmental and biological systems so we need good ways to characterize them



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CEINT
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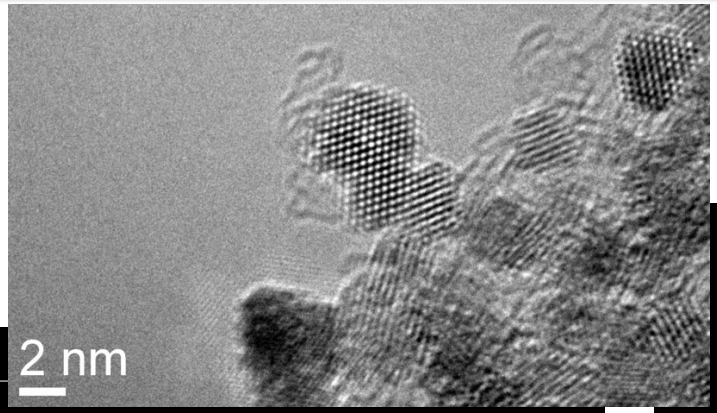
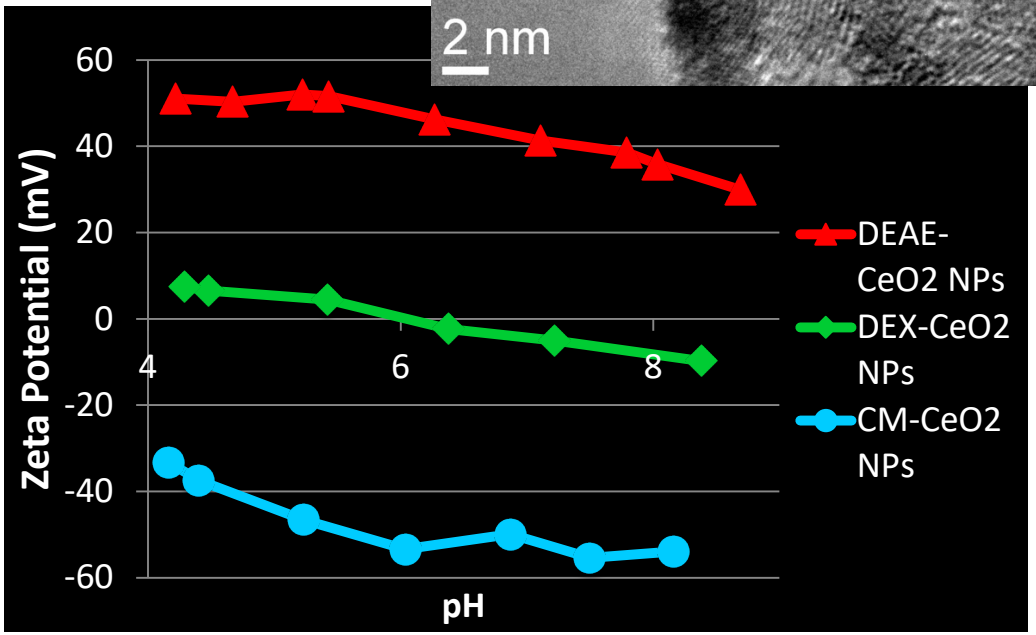
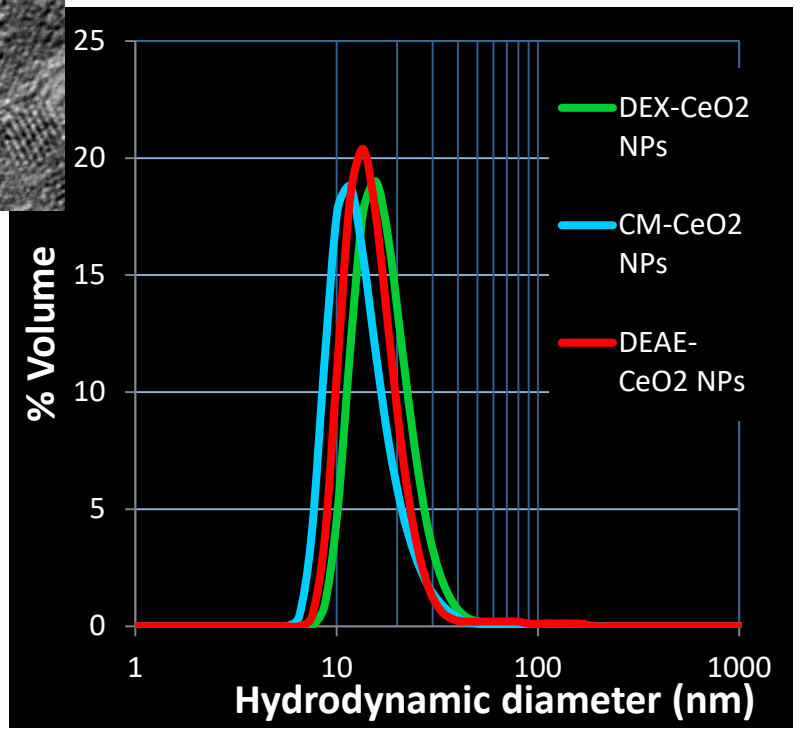
Nanoparticle functionalization- CeO_2 synthesis

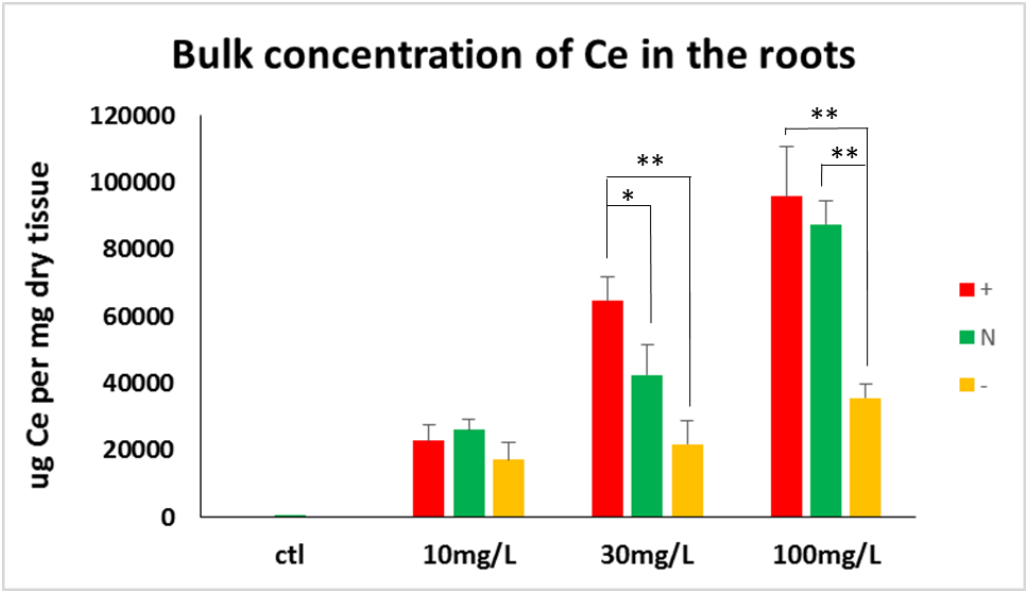


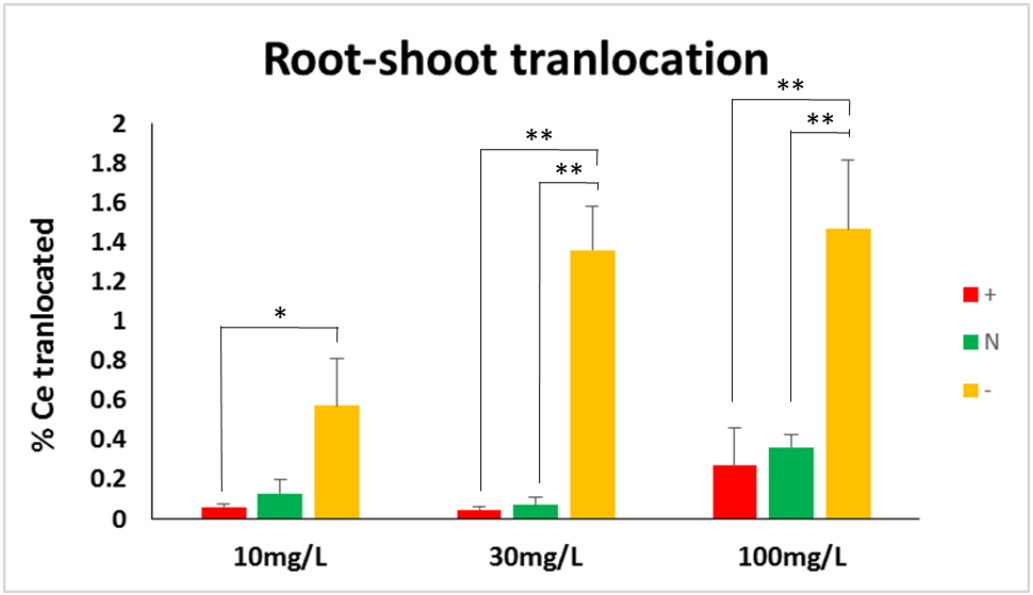




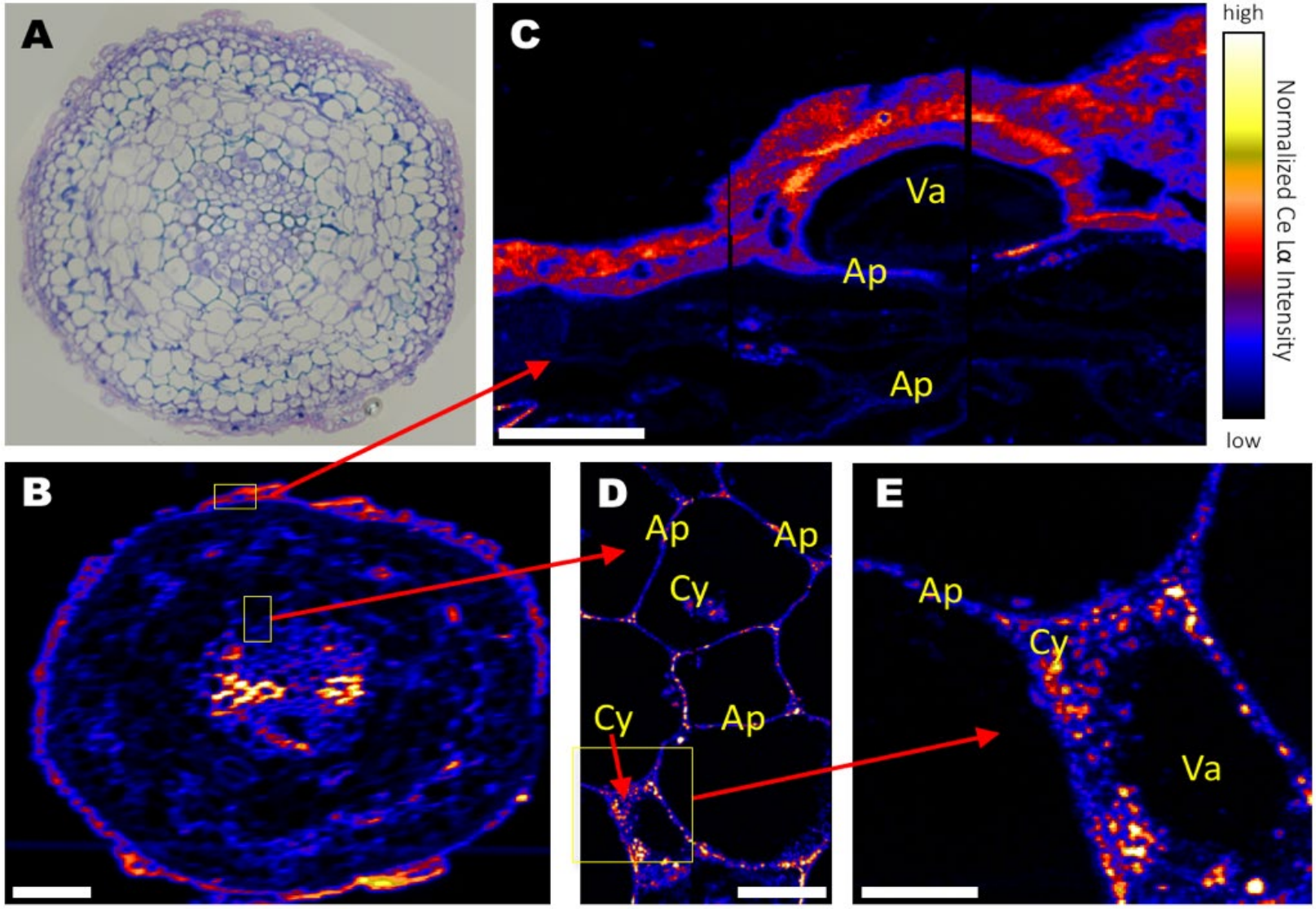
Diethylamioethyldextran (DEAE) – Positive charge
Dextran (DEX) - Neutral
Carboxymethyldextran (CM) –Negative charge

Lycopersicum solanum
cv Microtom

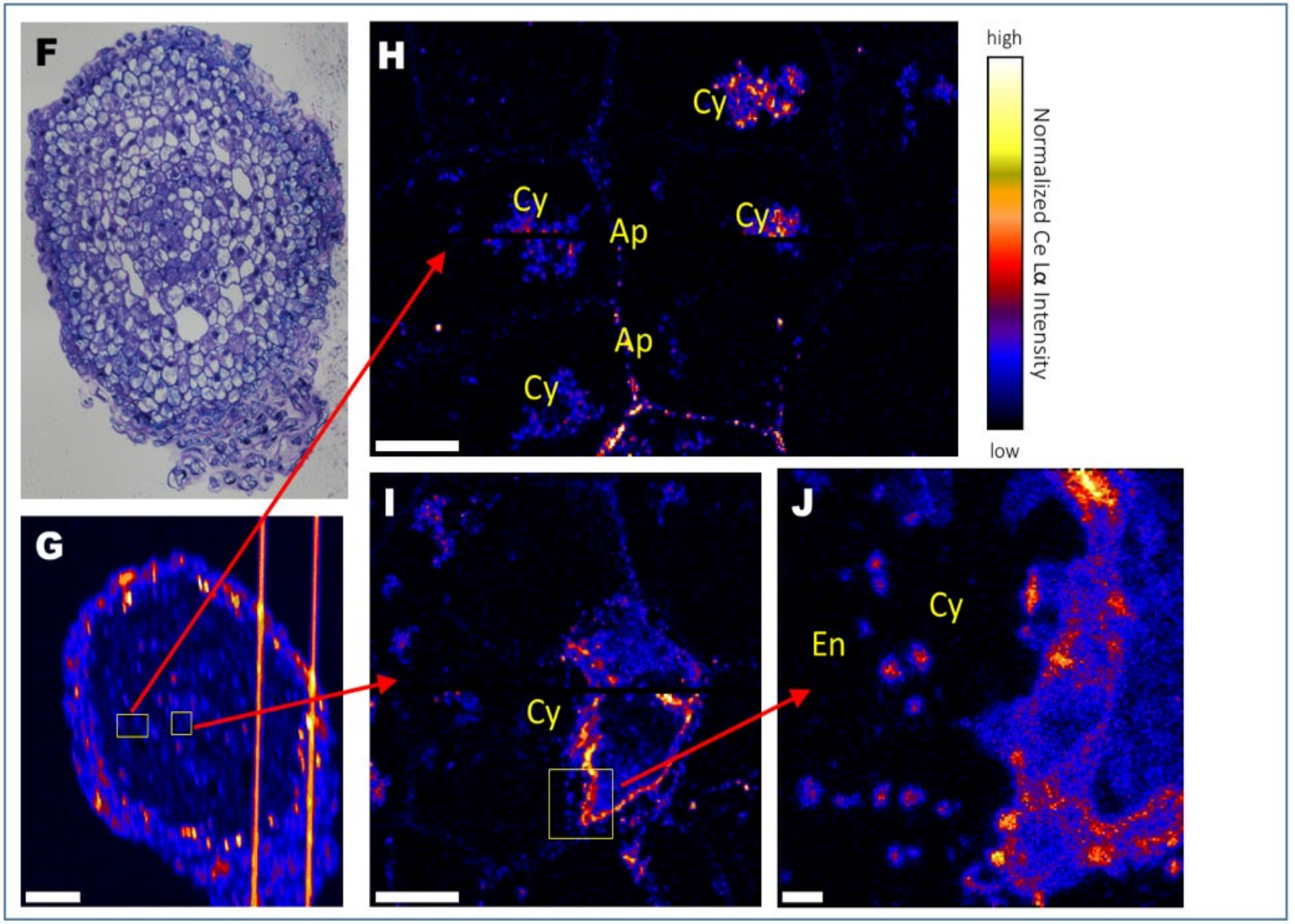




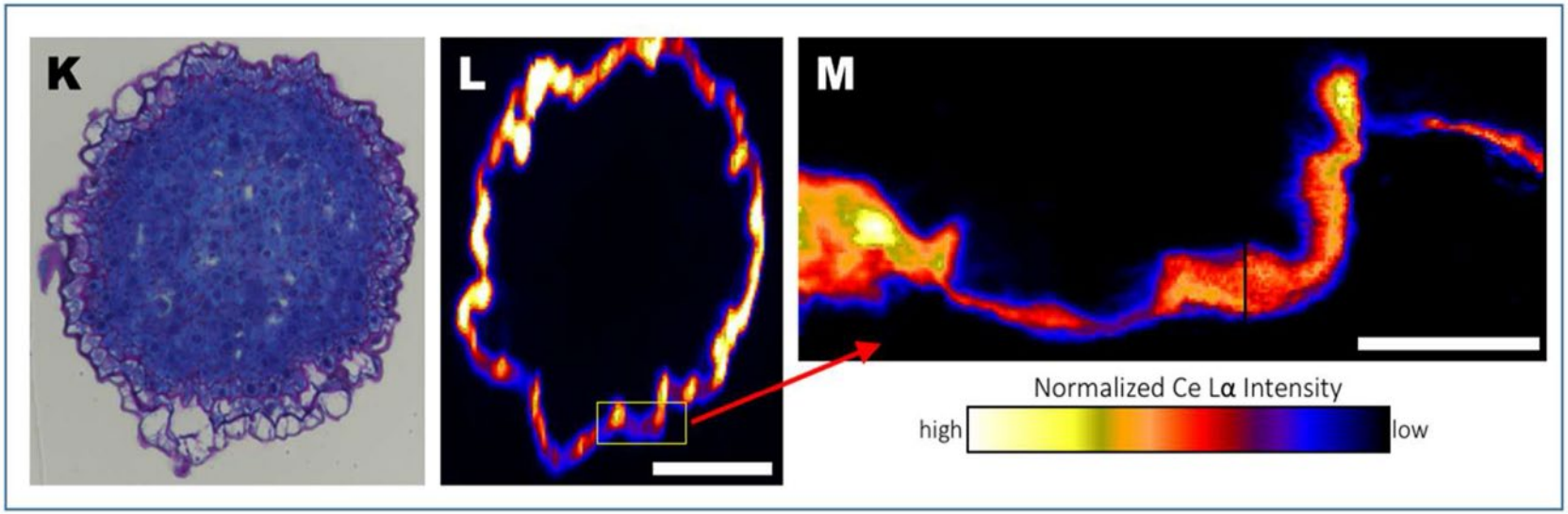
Dextran coated particles – neutral charge



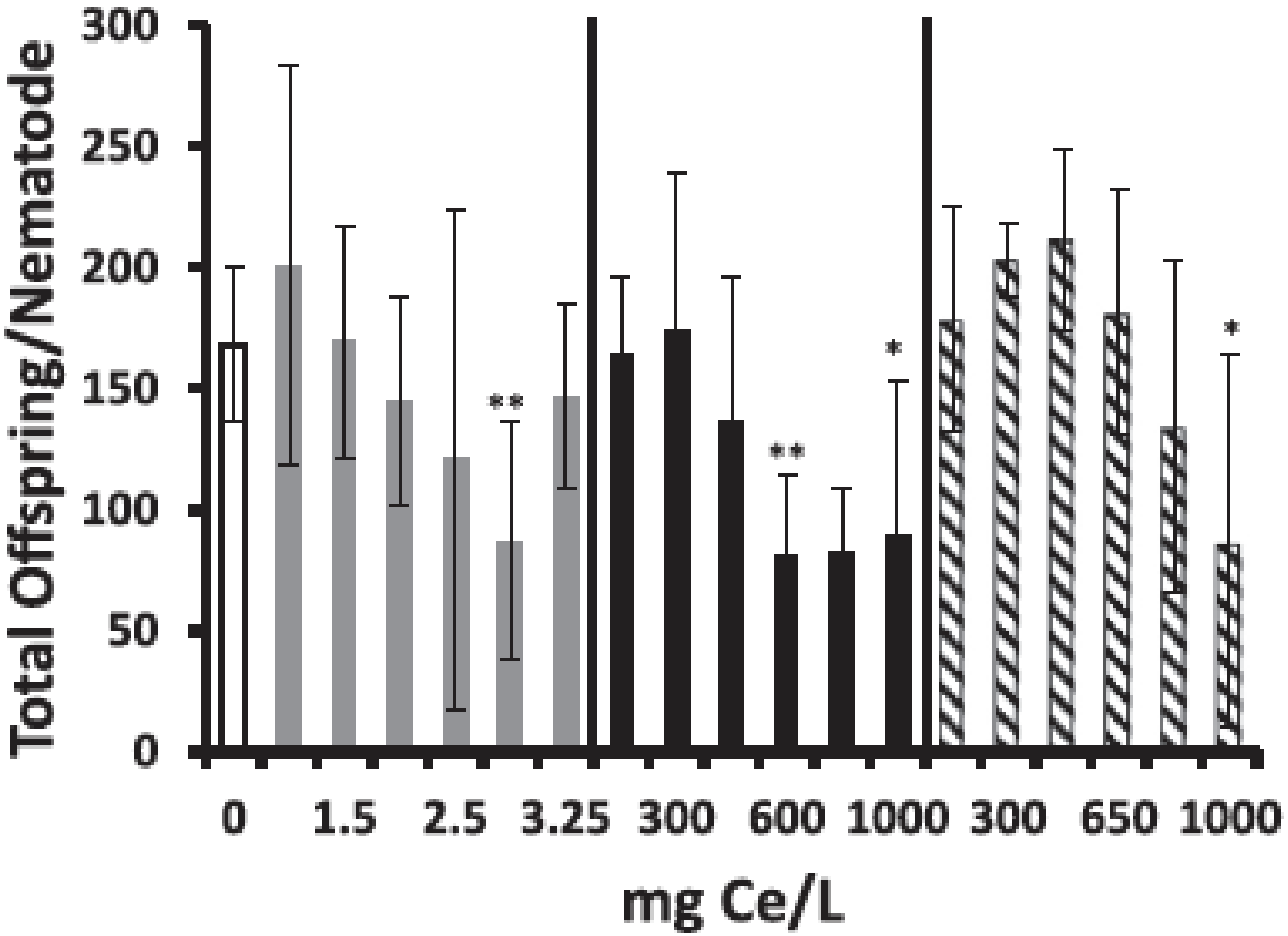
Carboxymethyldextran coated particles – negative charge



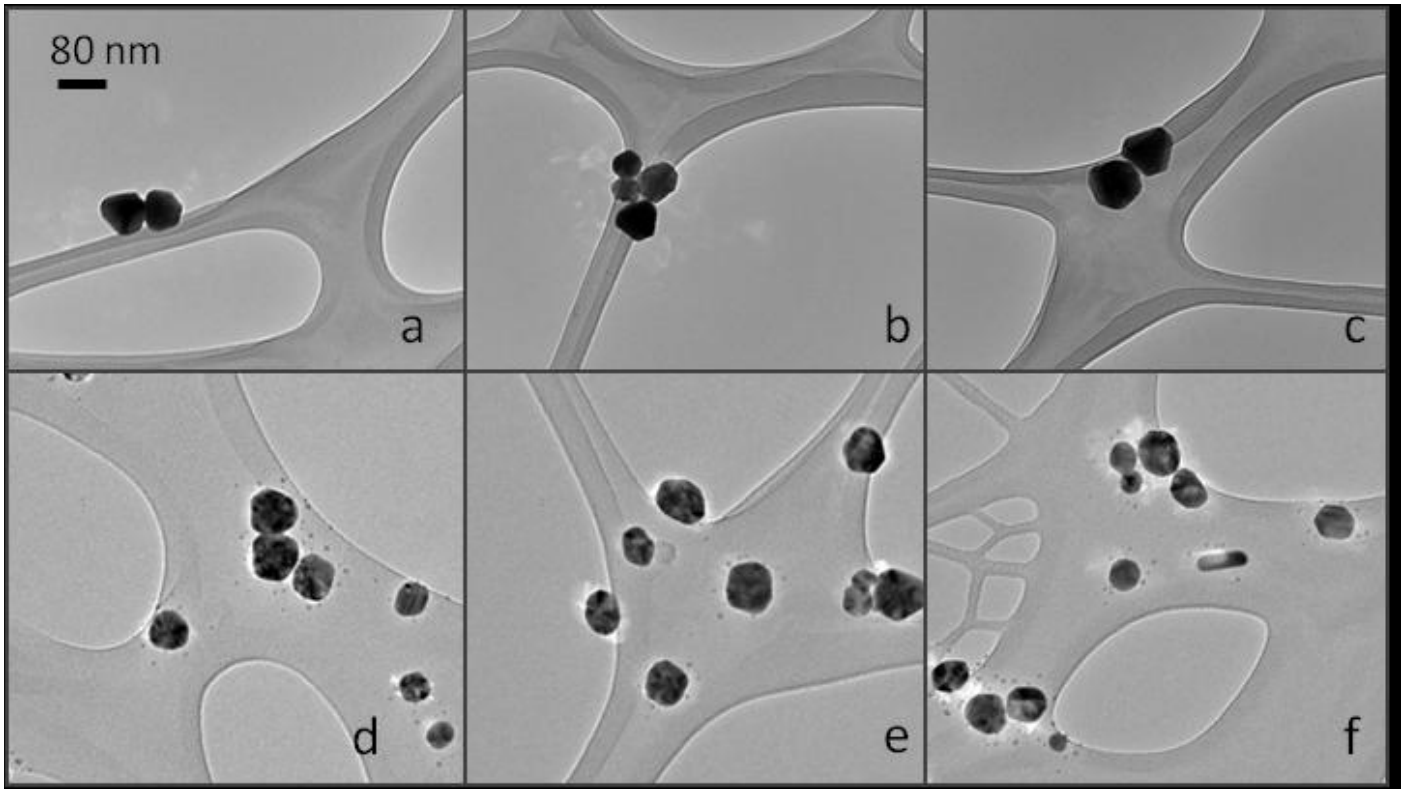
Diethylaminoethyldextran coated particles – positive charge



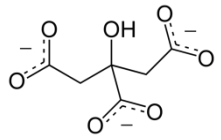
Reproductive Toxicity in *C. elegans*



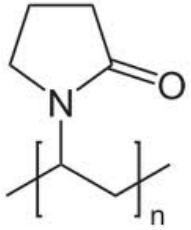
How do coatings affect the fate of Ag nanomaterials?

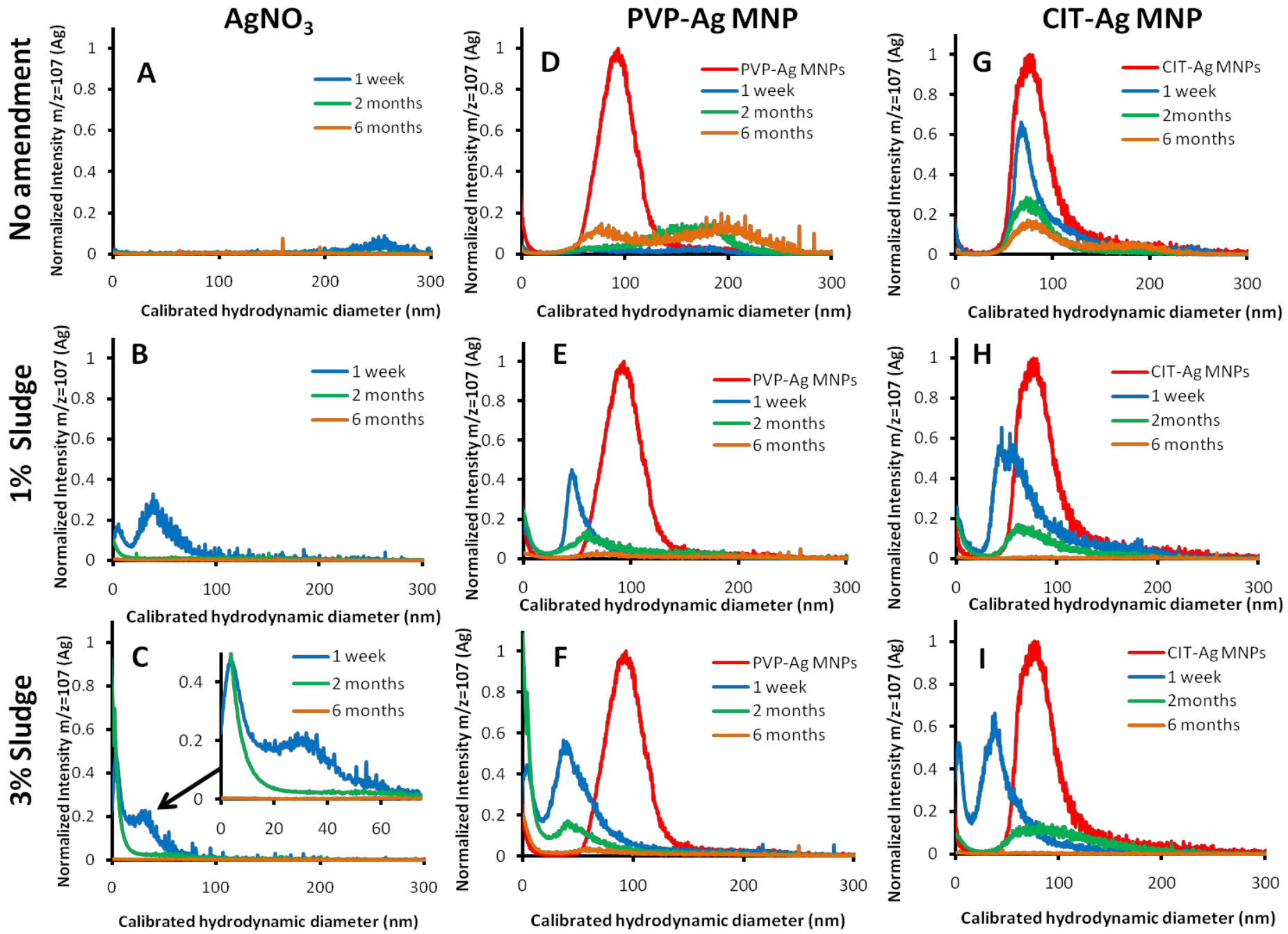


Citrate

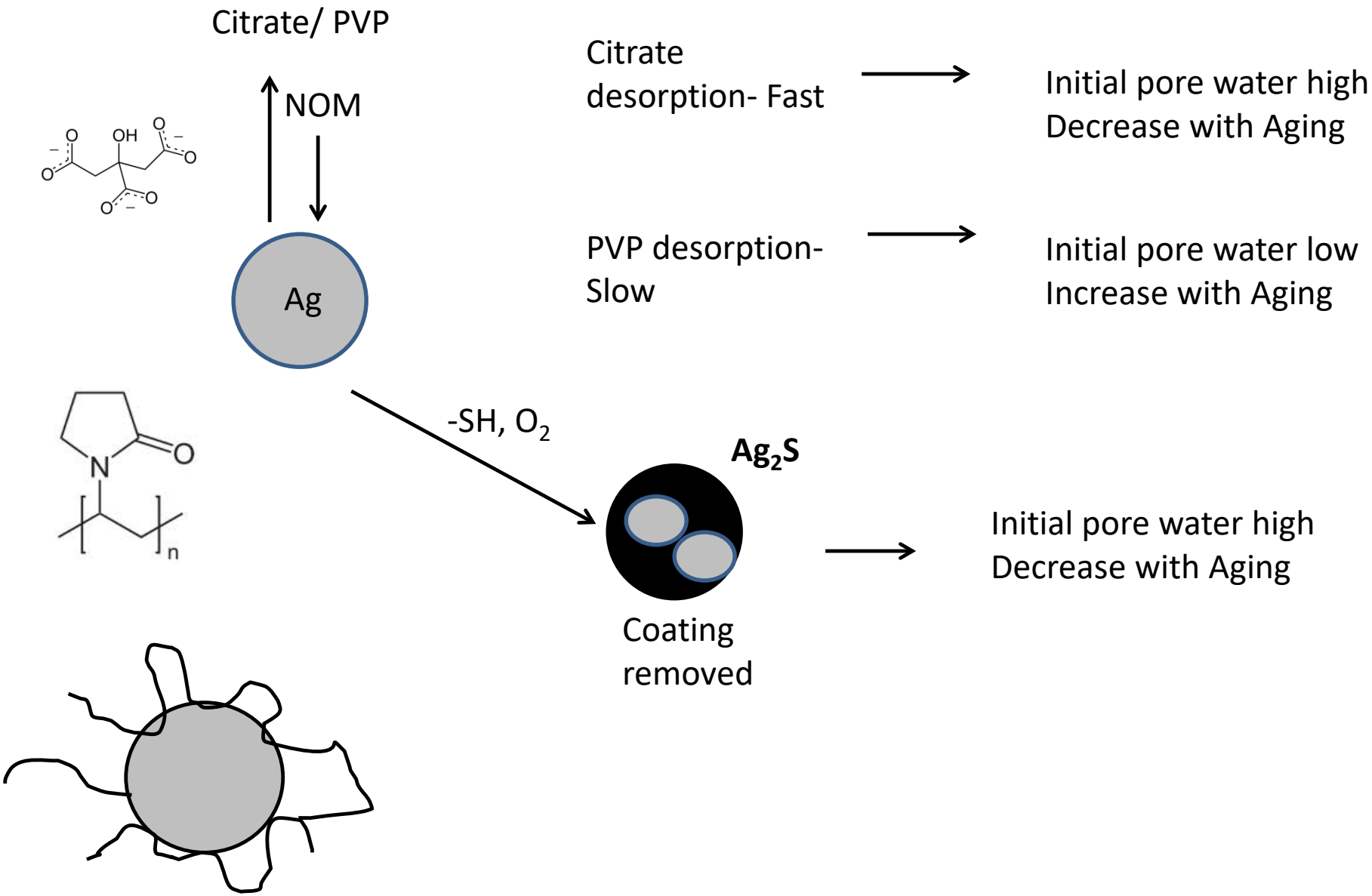


PVP – 55 kDa



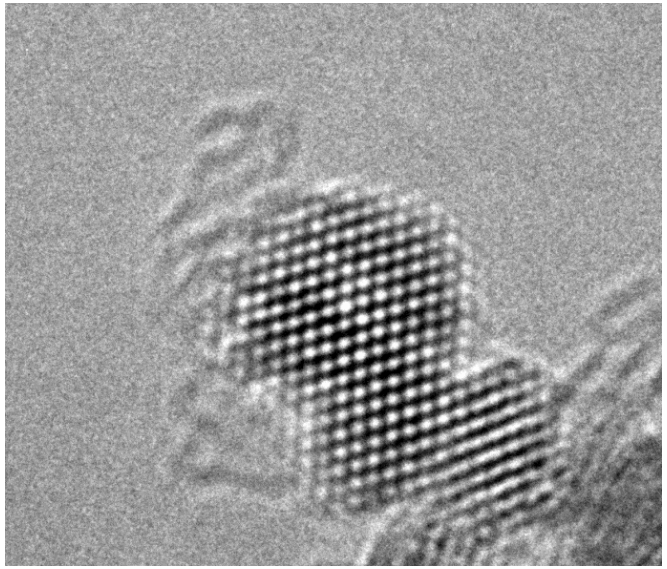


Whitley et al., 2014 Environmental Pollution

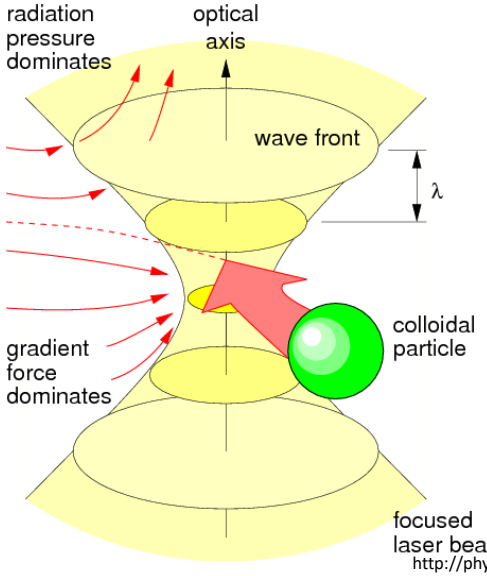

Citrate/ PVP
NOM
Ag
Citrate desorption- Fast
Initial pore water high
Decrease with Aging
PVP desorption- Slow
Initial pore water low
Increase with Aging
-SH, O_2
Ag_2S
Coating removed
Initial pore water high
Decrease with Aging

How could we characterize the coatings in complex media?

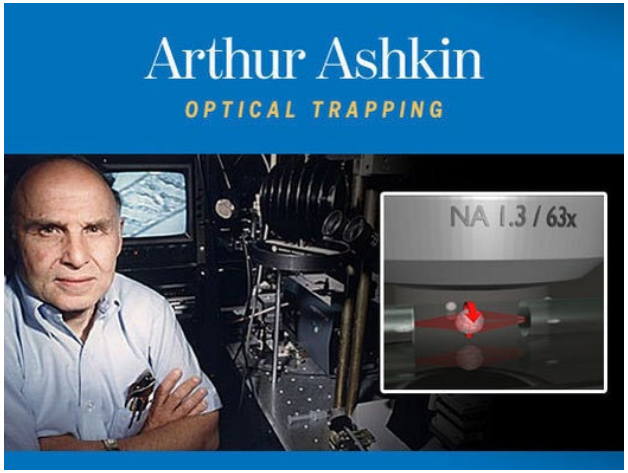
- Step 1- Isolate (individual) particles
- Step 2- Measure particle size
- Step 3- Collect spectral data (MS, FTIR, Raman, UV-Vis).
- Step 4- Analyze the spectral data (hardest part; machine learning/AI)



Optical trapping - spectroscopy



http://physics.nyu.edu/grierlab/hot.html



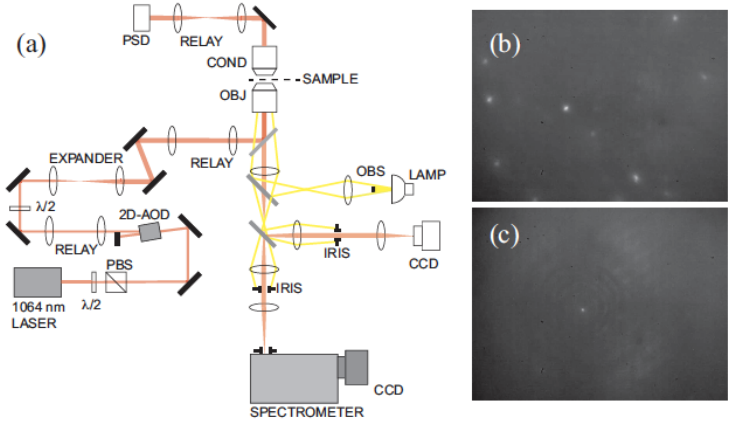


Fig. 1. (a) Optical tweezers setup that incorporates dark-field microscopy / spectroscopy. The illuminating light is formed into a ring by placing a custom-made block after the light source. The image of this ring is projected onto the sample; its reflection is blocked from entering the CCD camera by using an aperture, allowing only the scattered light to pass. (b) Dark field images of freely moving 200nm particles, (c) a trapped 100nm particle.

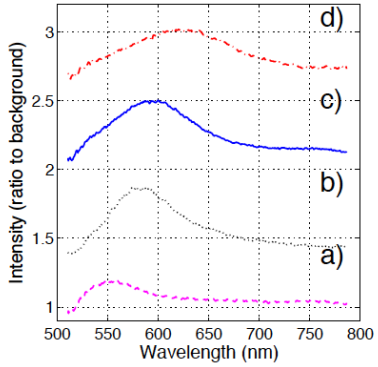
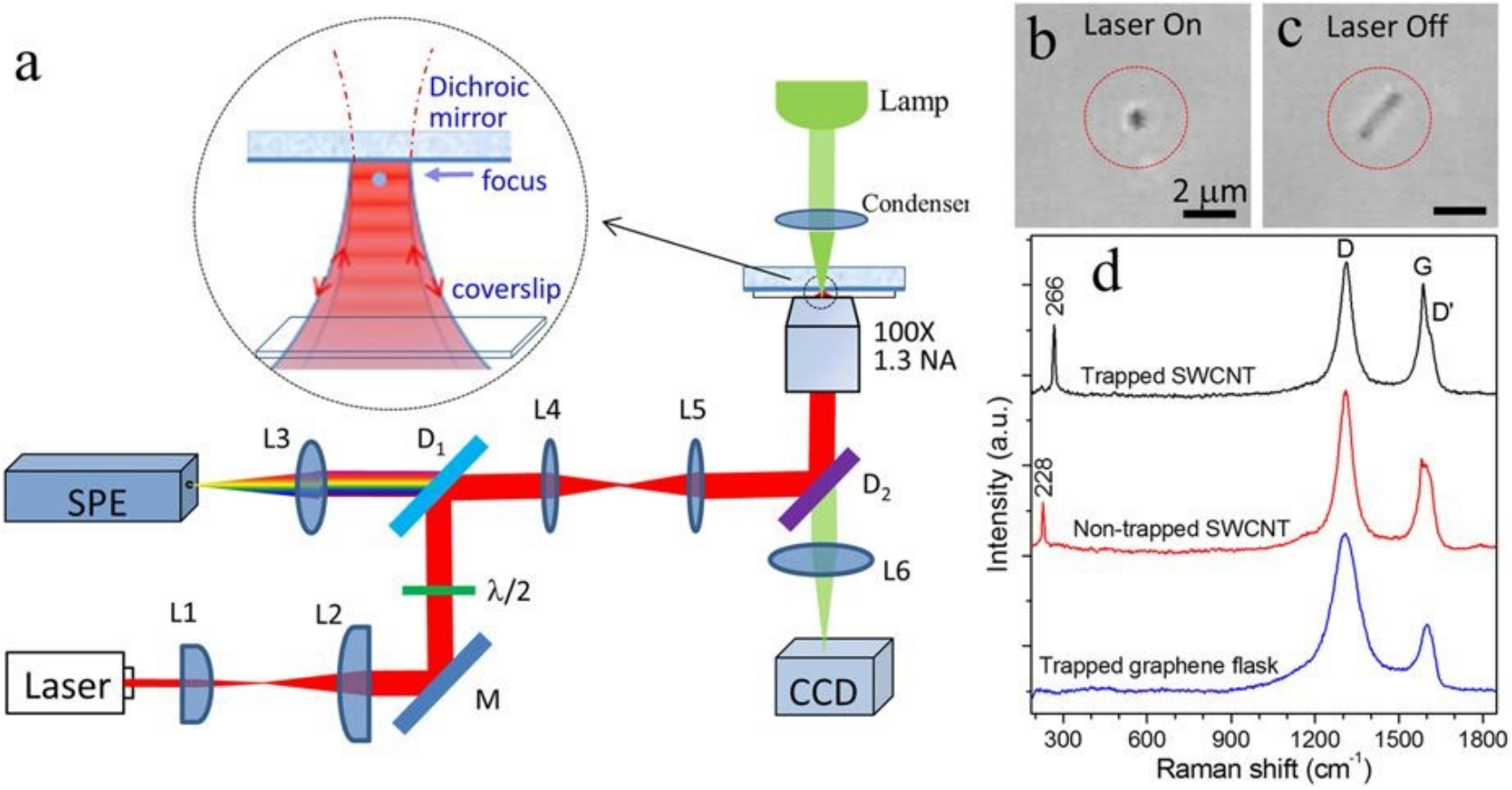


Fig. 3. Spectra obtained from trapped gold particles found in samples with nominal sizes 60, 80, 100 and 150nm (a-d). In the case of (d) the peak is at a shorter wavelength than expected, however, this can be explained by the observed distribution of particle sizes within each sample. With increasing particle size a redshift and broadening of the spectra can be seen.

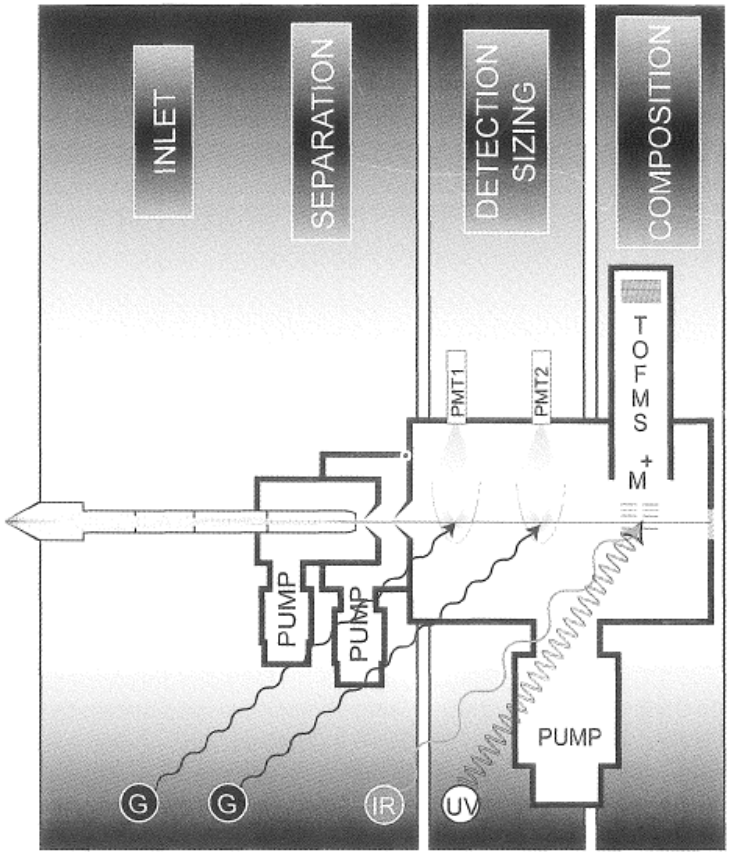
Pearce, K.; Wang, F.; Reece, P. J., Dark-field optical tweezers for nanometrology of metallic nanoparticles. *Opt Express* **2011,** *19*, (25), 25559-25569.

Optical trapping of a SWCNT with Raman spectroscopy



Wu, M.-y.; Ling, D.-x.; Ling, L.; Li, W.; Li, Y.-q., Stable optical trapping and sensitive characterization of nanostructures using standing-wave Raman tweezers. *Scientific reports* **2017,** *7*, 42930.

Single particle laser ablation TOF MS – ”SPLAT”



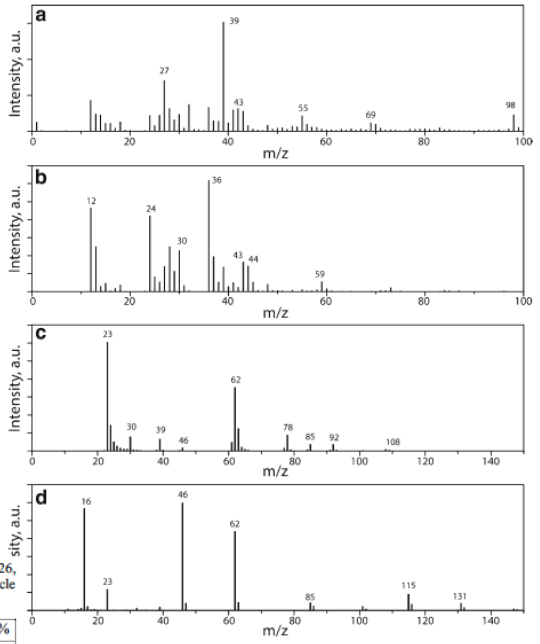
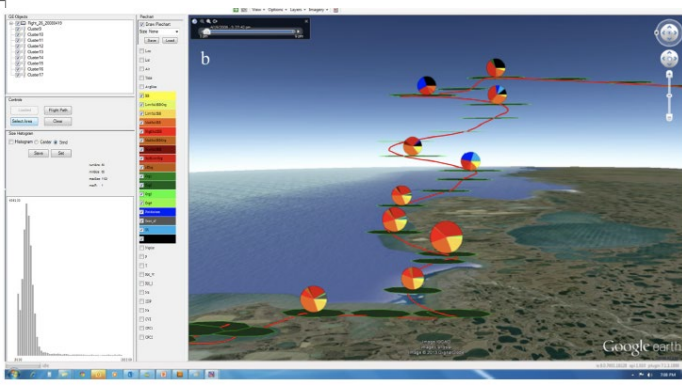


Table 1. A legend of the compositions of particle classes observed during F26, the colors used to represent them in Figures 3, 4 and 6, their measured particle densities, and sulfate weight fraction, measured with uncertainties of ±5%

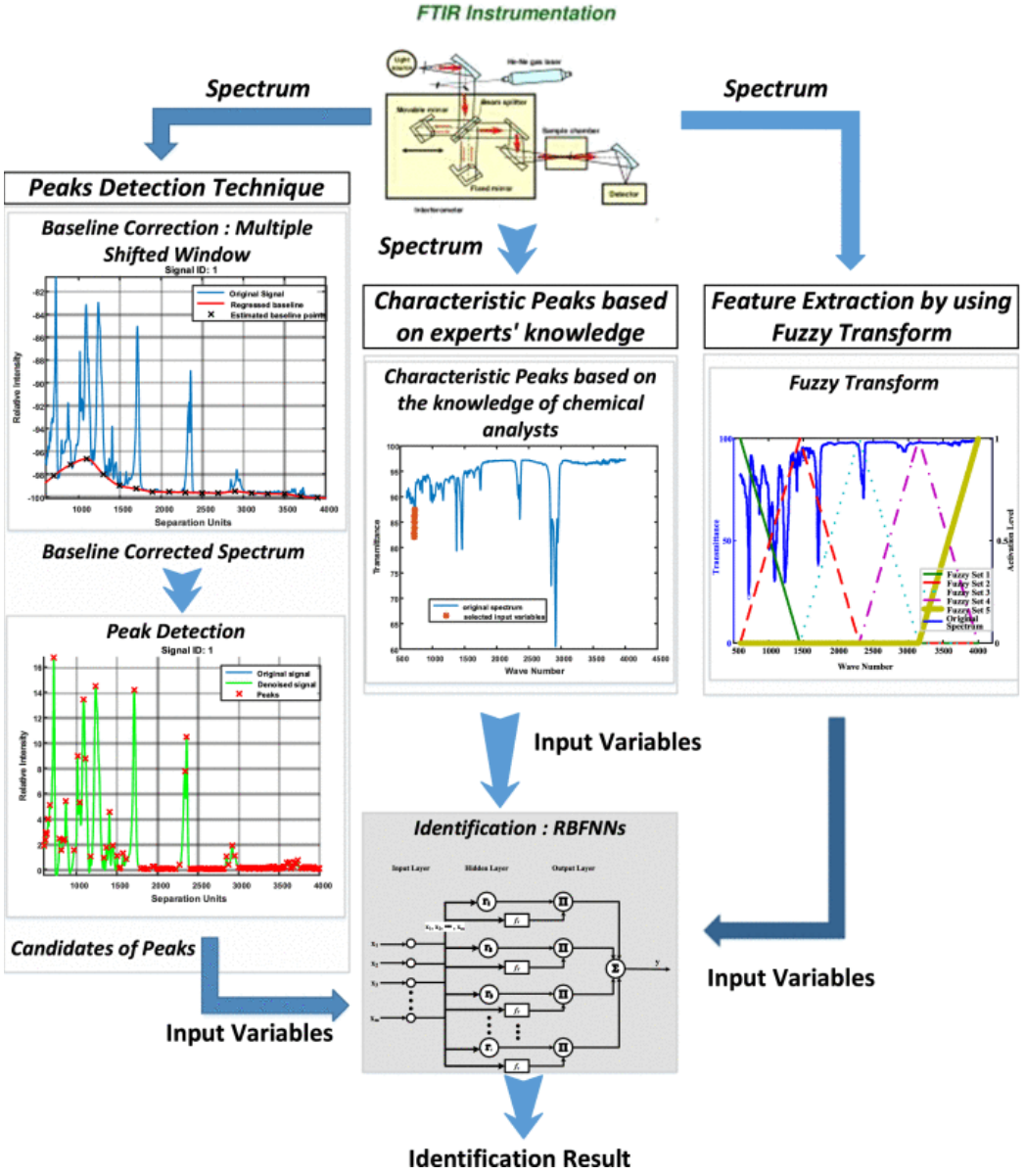
Color	Class	Density, g•cm^{-3}	Sulfate *WF*, %
	BB	1.32	0
	LowSulfBBorg	1.35	15
	LowSulfBB	1.38	15
	MedSulfBB	1.47	40
	HighSulfBB	1.58	60
	SulfBBorg	1.45	40
	SootSulfBB	-	-
	SulfLowOrg	1.47	50
	SulfOrg	1.30	20
	Org1	1.22	0
	Org2	1.24	0
	Org3	1.24	0
	Org4	1.24	0
	Pyridinium ion	1.5	0
	Soot_org	1.25	0
	SS	1.5	0
	Mineral dust	-	-



Alla Zelenyuk & Dan Imre (2005) Single Particle Laser Ablation Time-of-Flight Mass Spectrometer: An Introduction to SPLAT, Aerosol Science and Technology, 39:6, 554-568, DOI: 10.1080/027868291009242

Zelenyuk, A.; Imre, D.; Wilson, J.; Zhang, Z.; Wang, J.; Mueller, K., Airborne Single Particle Mass Spectrometers (SPLAT II & miniSPLAT) and New Software for Data Visualization and Analysis in a Geo-Spatial Context. *Journal of The American Society for Mass Spectrometry* **2015,** *26*, (2), 257-270.

Neural networks for compound identification



Roh et al IEEE TRANSACTIONS ON INDUSTRIAL INFORMATICS, VOL. 14, NO. 5, MAY 2018

Summary and Research Needs

- Coatings have a dominant influence on nanomaterial behavior in environmental and biological systems.
- Tools for characterizing coatings in situ have lagged far behind tools for characterizing core chemistry.
- Instrumentation which can manipulate single particles in complex media for collection of spectral data coupled with advanced computational methods is one possible path forward.