

On the importance of atom probe tomography for the development of new nanoscale devices

Thales Borrelly* and Alain A. Quivy
Institute of Physics – University of São Paulo

Tao-Yu Huang, Yu-Chen Yang, and Rachel S. Goldman
Materials Science & Engineering – University of Michigan

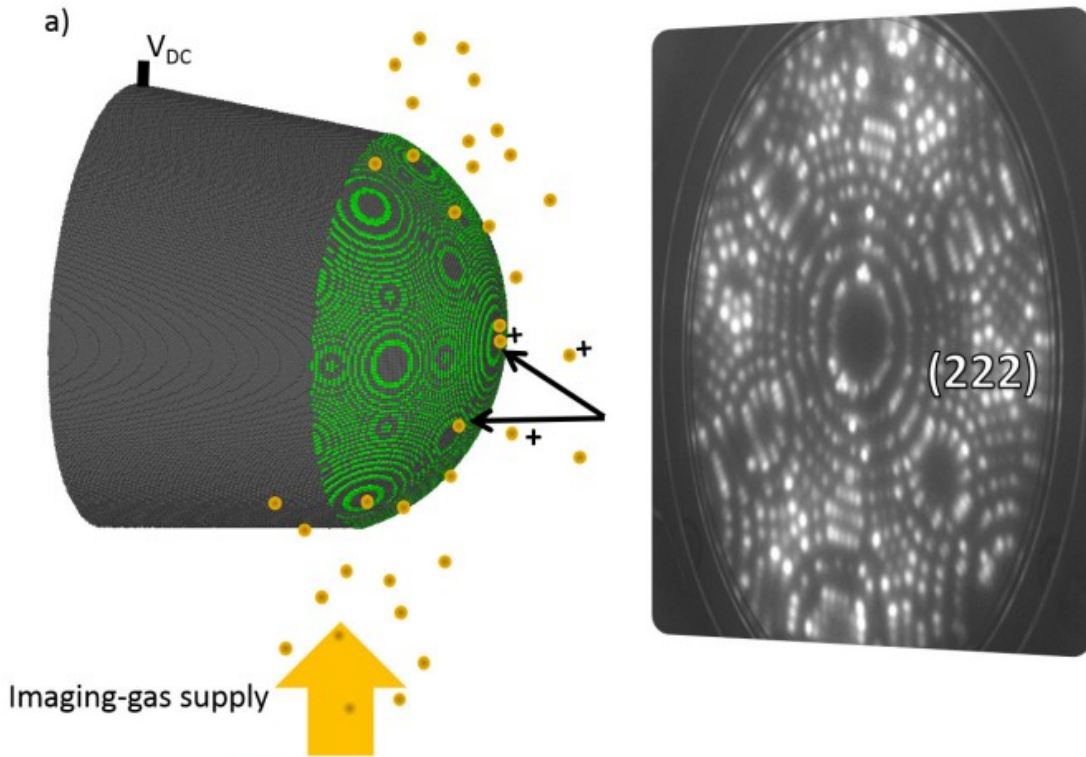
*email: thales.santos@usp.br

Overview

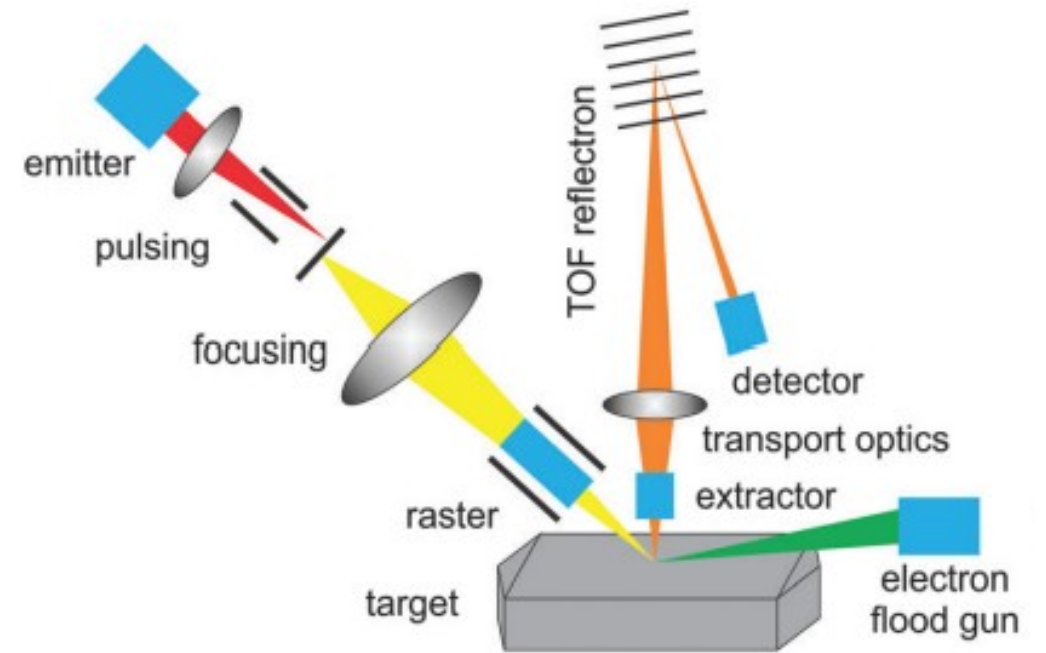
- Fairly rare: 100 systems worldwide (reported in 2020 [1]).
- Unique. Provides spatial distribution of all elements with sub-nanometer resolution.
- Expensive. Requires complex sample preparation.
- Extremely useful for developing nanostructured devices.

Working principle

Field ion microscopy (FIM)



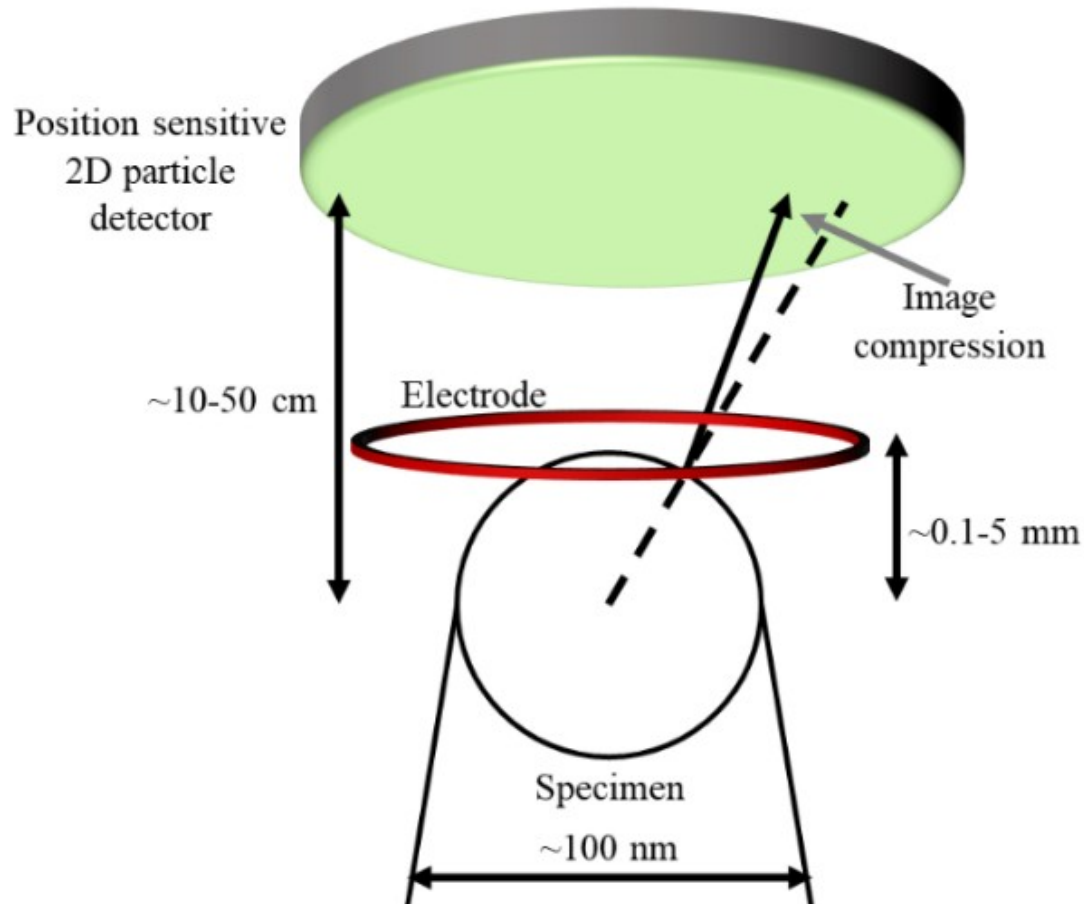
Time-of-flight secondary ion mass spectroscopy (ToF SIMS)



Shyam Katnagallu *et al* 2018 *J. Phys. D: Appl. Phys.* **51** 105601

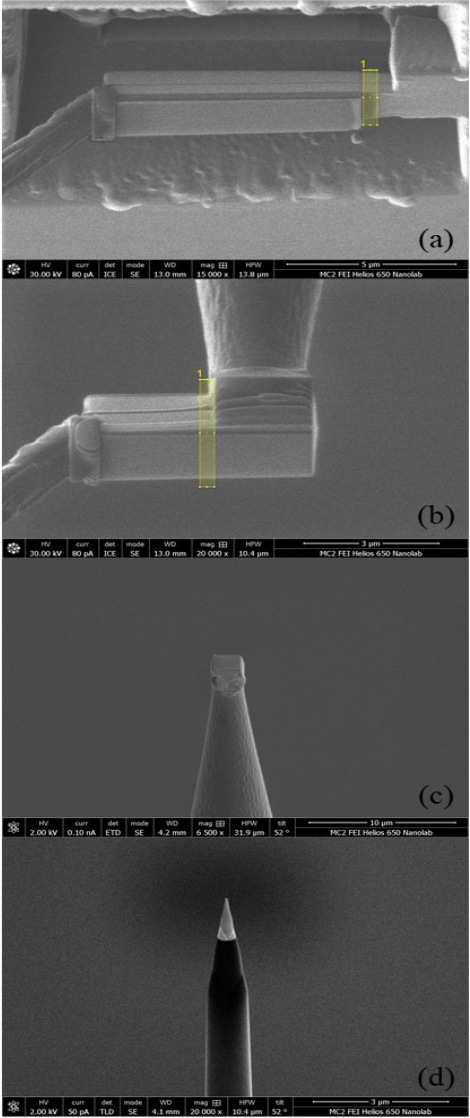
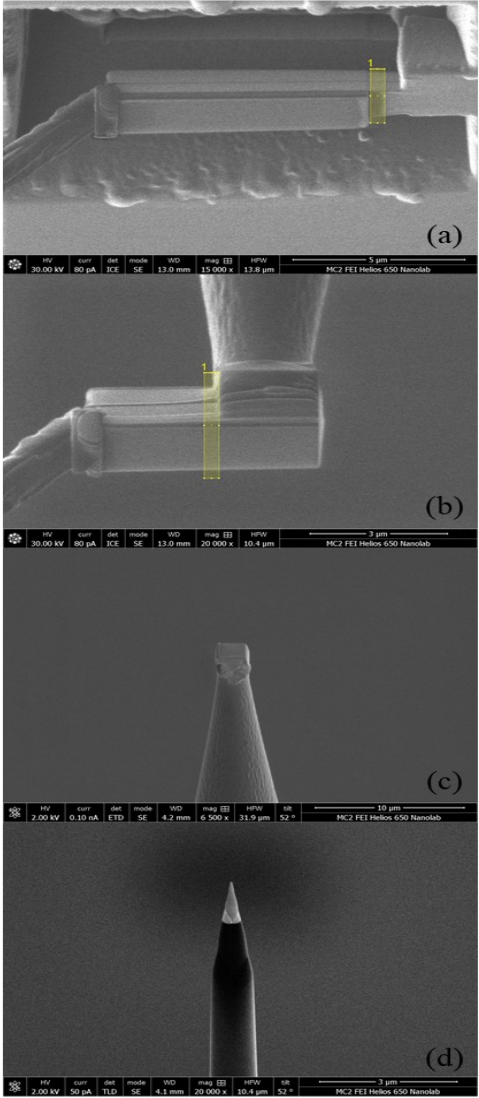
Jan P. Hofmann *et al*, *Phys. Chem. Chem. Phys.*, 2014,16, 5465-5474

Working principle

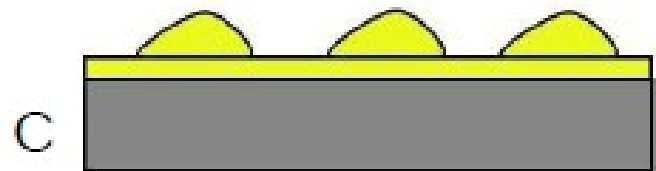
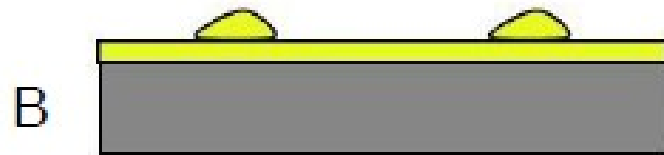


- Sample is a truncated cone.
- Sample is evaporated by pulsed laser or voltage pulses.
- Evaporated particles are accelerated and detected by a 2D position-sensitive ToF mass spectrometer.
- Raw data: $\sim 10^7$ particles identified by (x, y, t) and mass-to-charge ratio.
- Atom-by-atom reconstruction of sample.

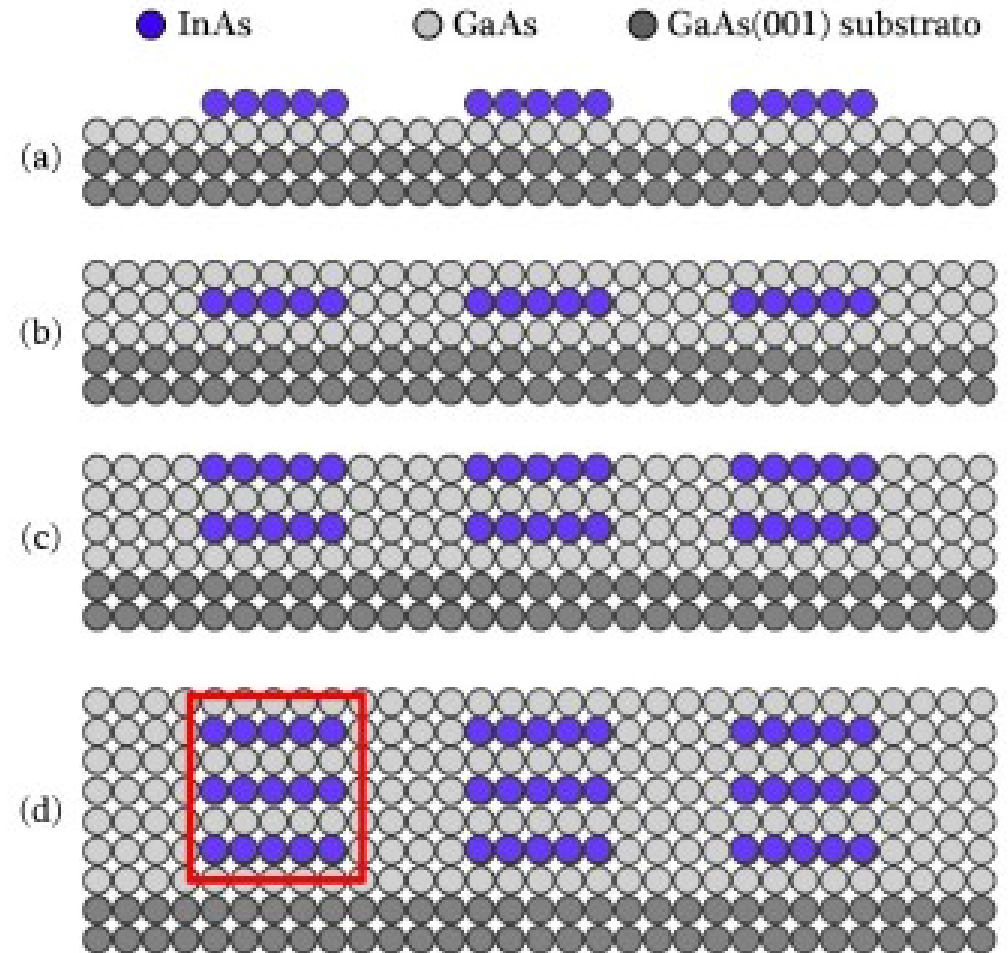
Sample preparation – SEM/FIB



Analysis: InAs/GaAs quantum dots

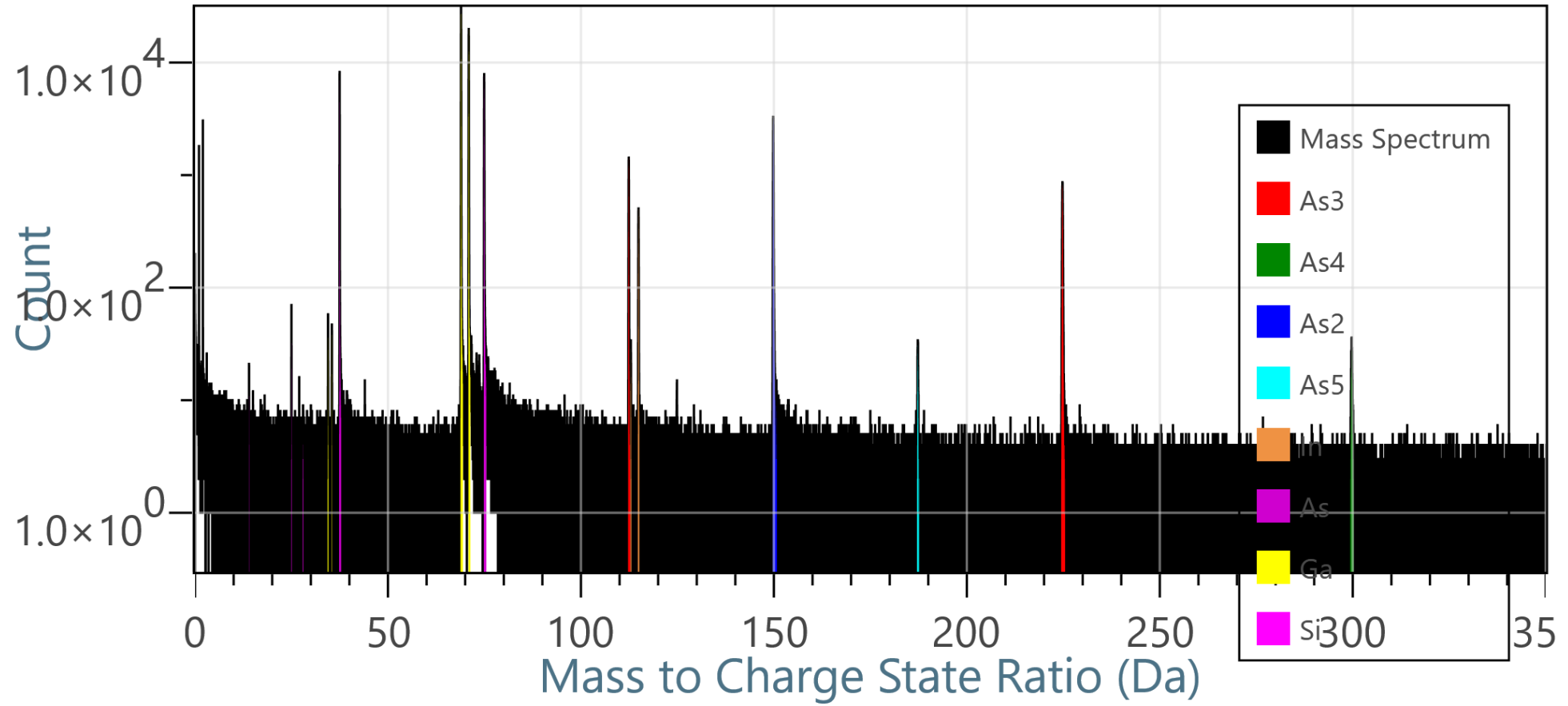


Stranski-krastanov quantum dots
SKQDs

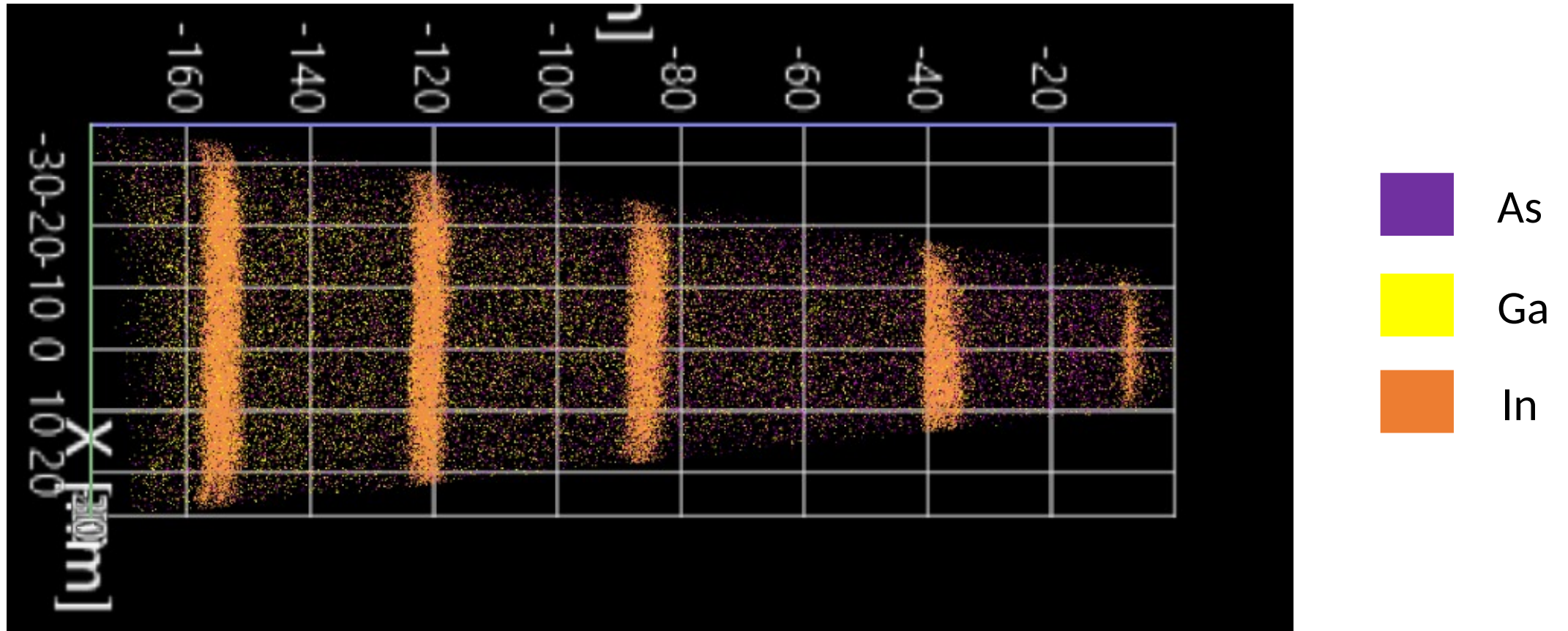


Submonolayer quantum-dots
SMLQDs

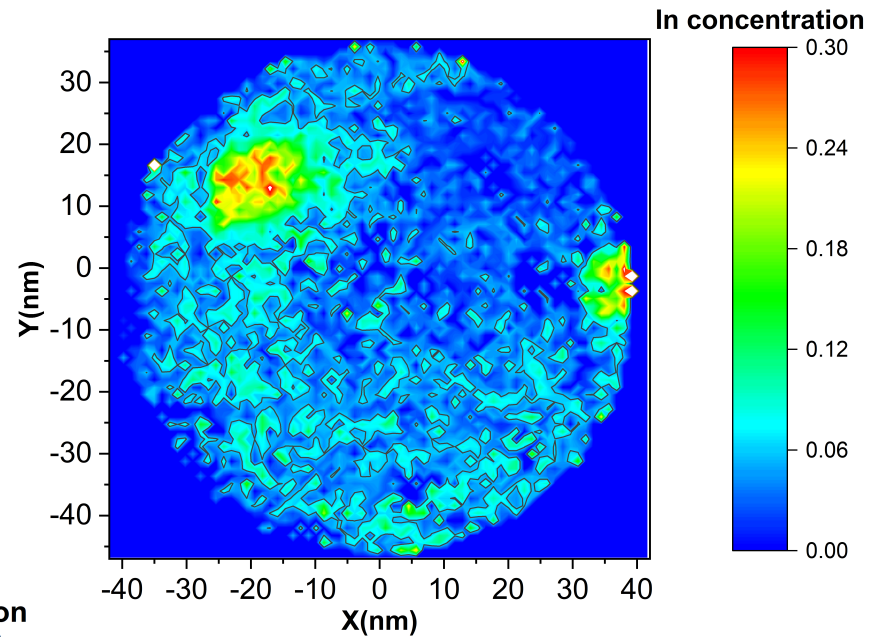
Analysis: mass-to-charge ratio identification



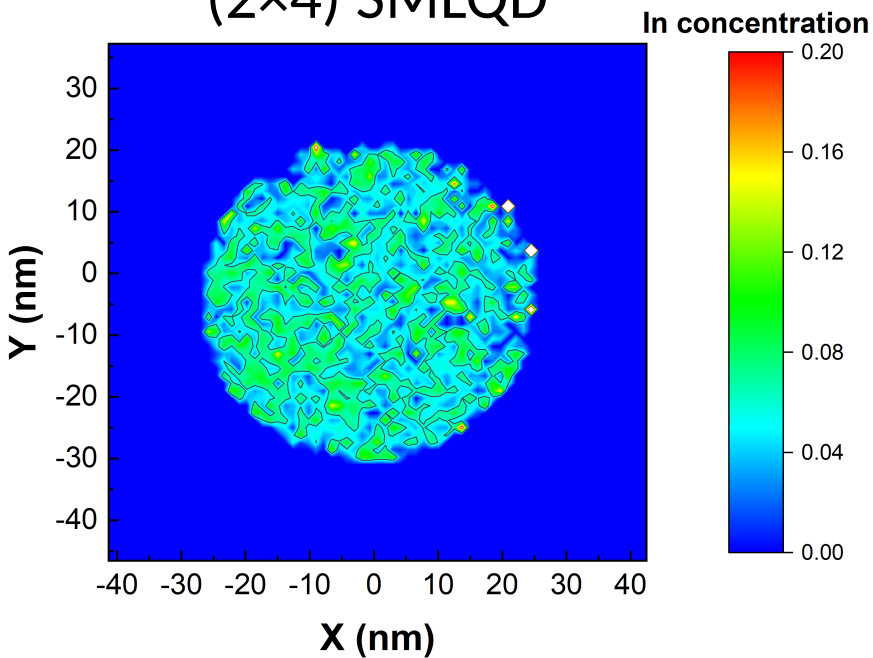
Analysis: reconstructed image



2D contour plot

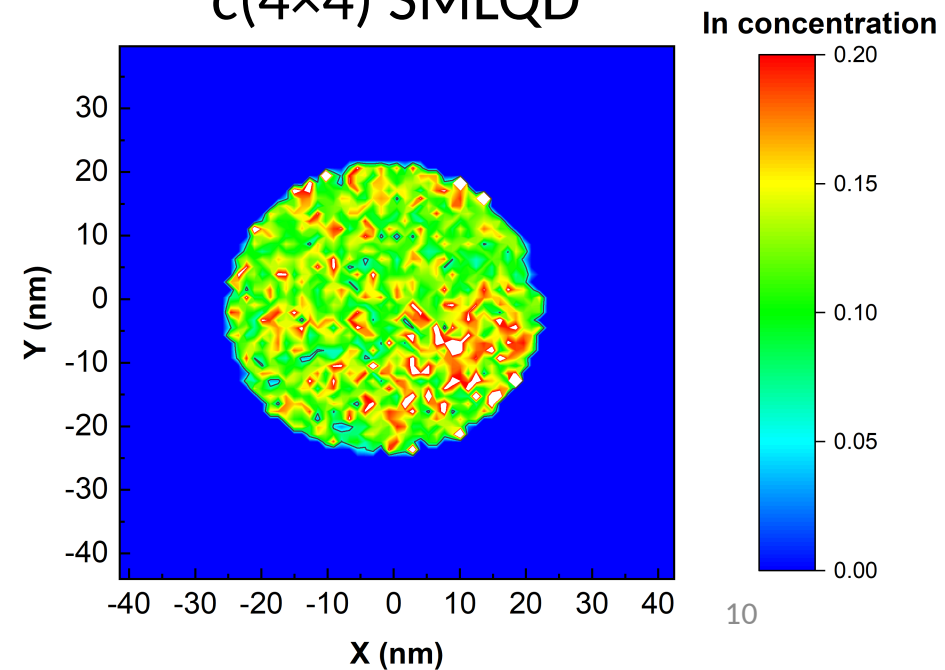


(2×4) SMLQD

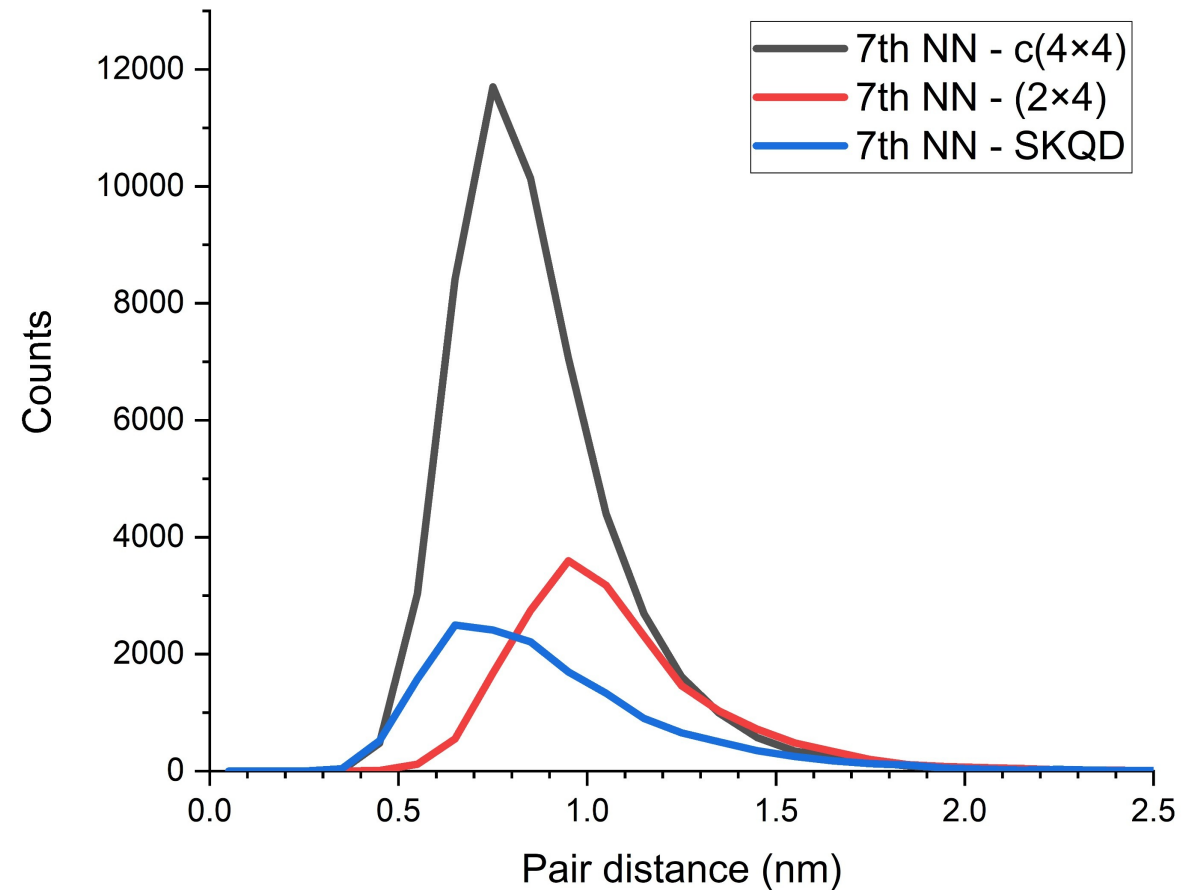
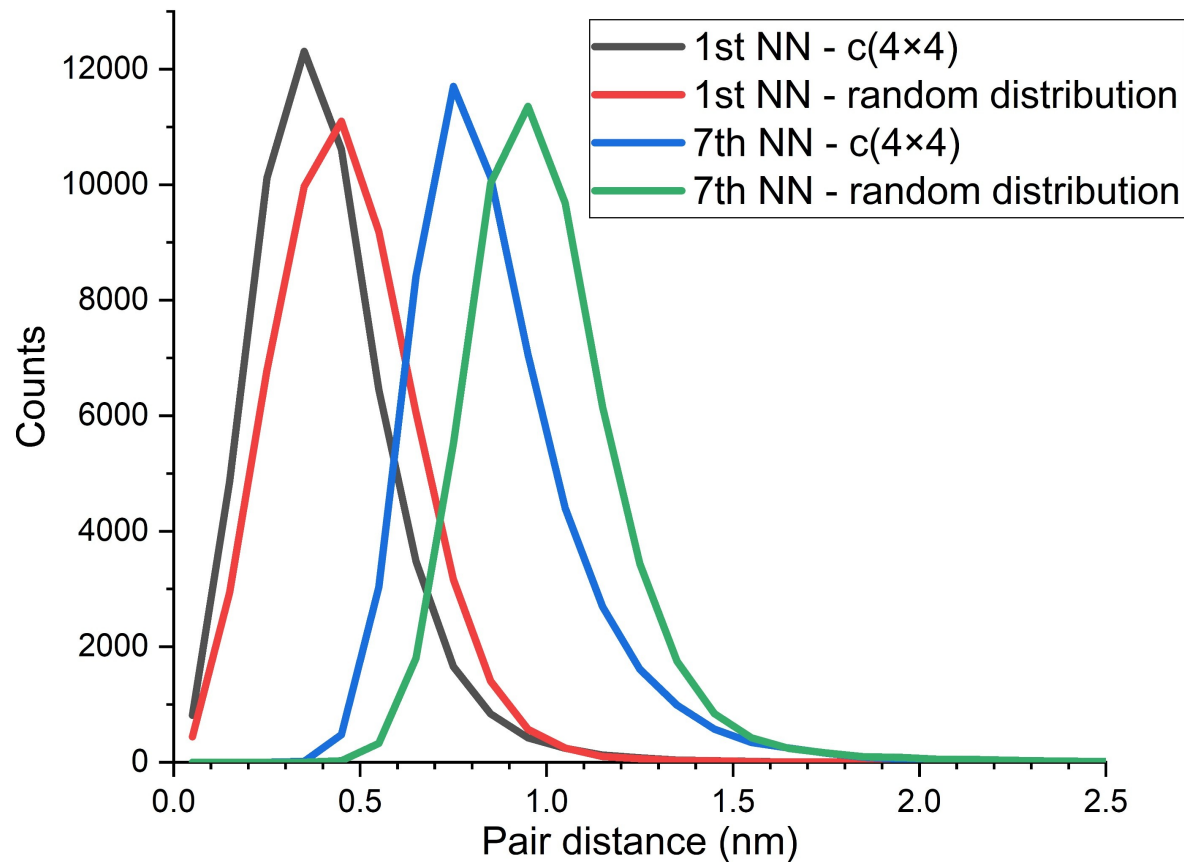


SKQD

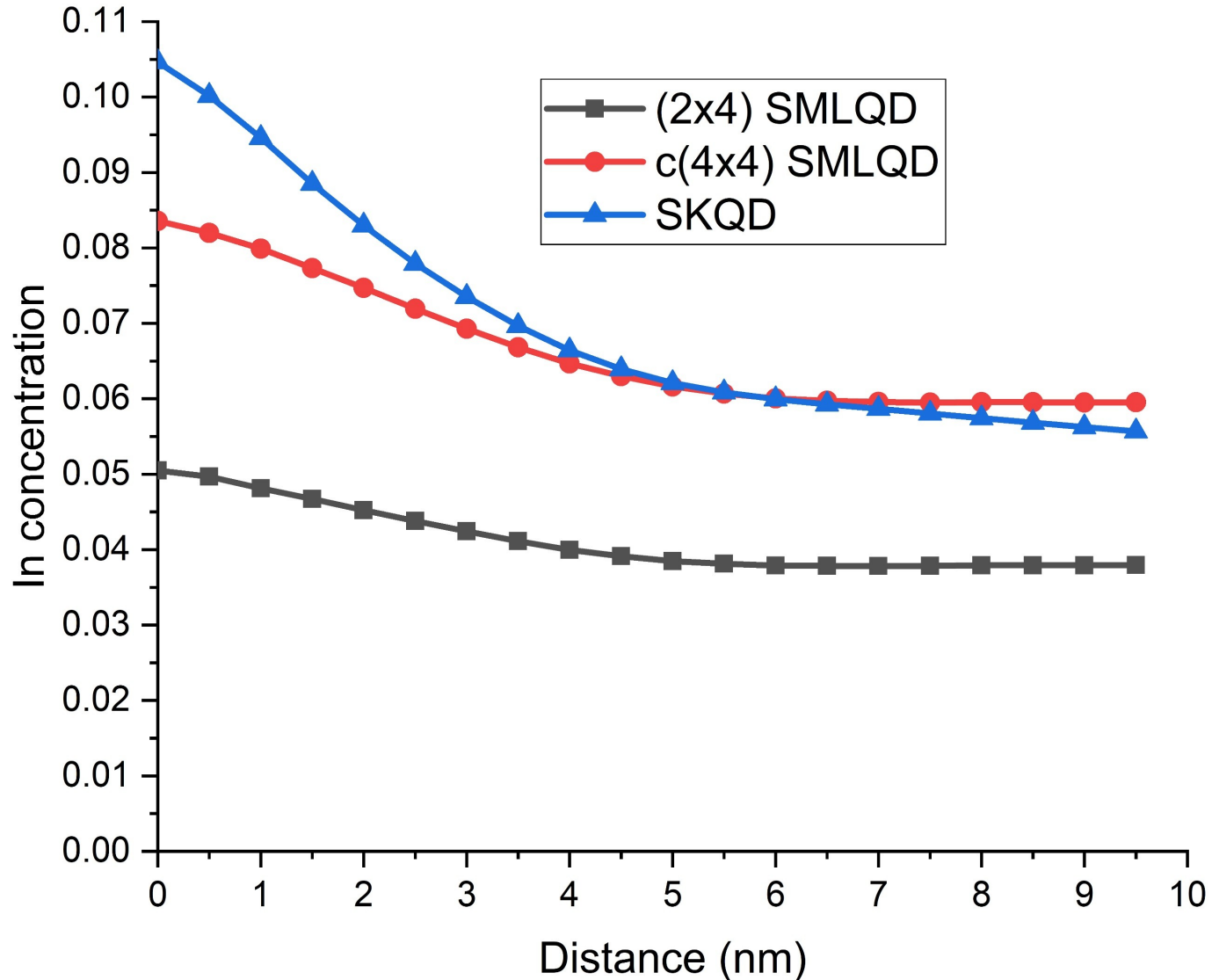
c(4×4) SMLQD



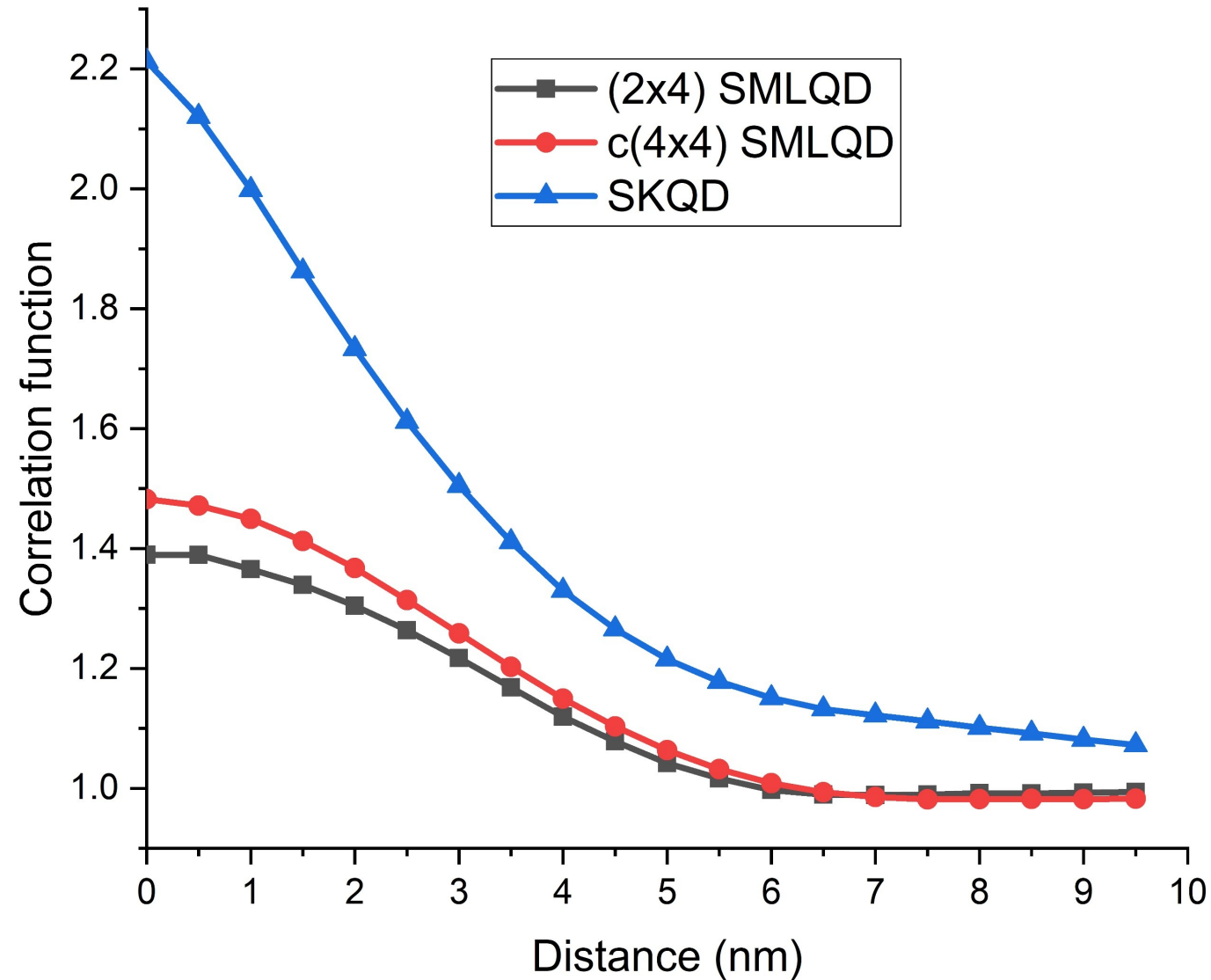
Nearest neighbor analysis: Existence of clusters



Radial distribution analysis: Composition distribution

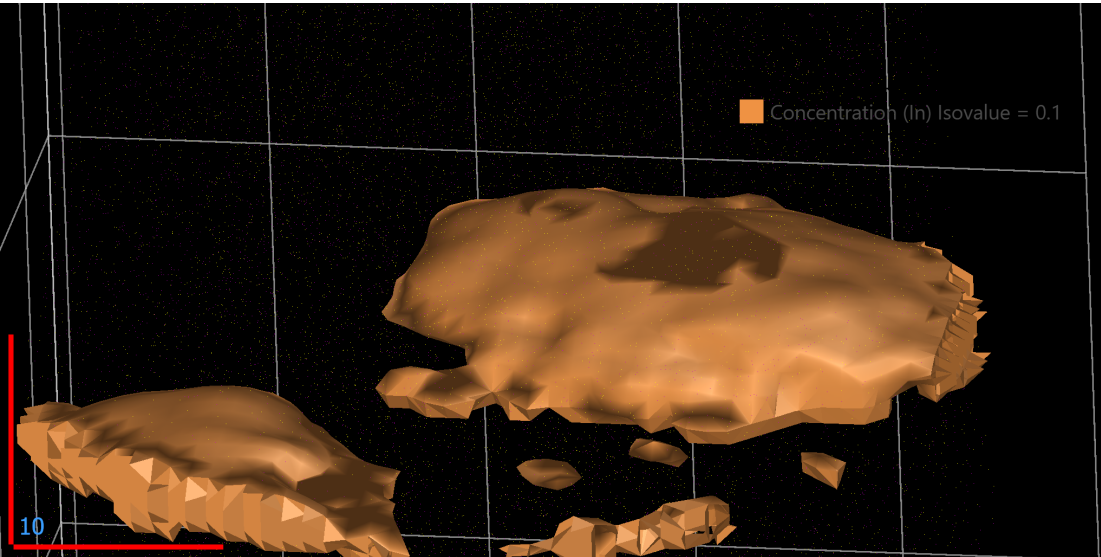


Correlation function: Degree of clusterization

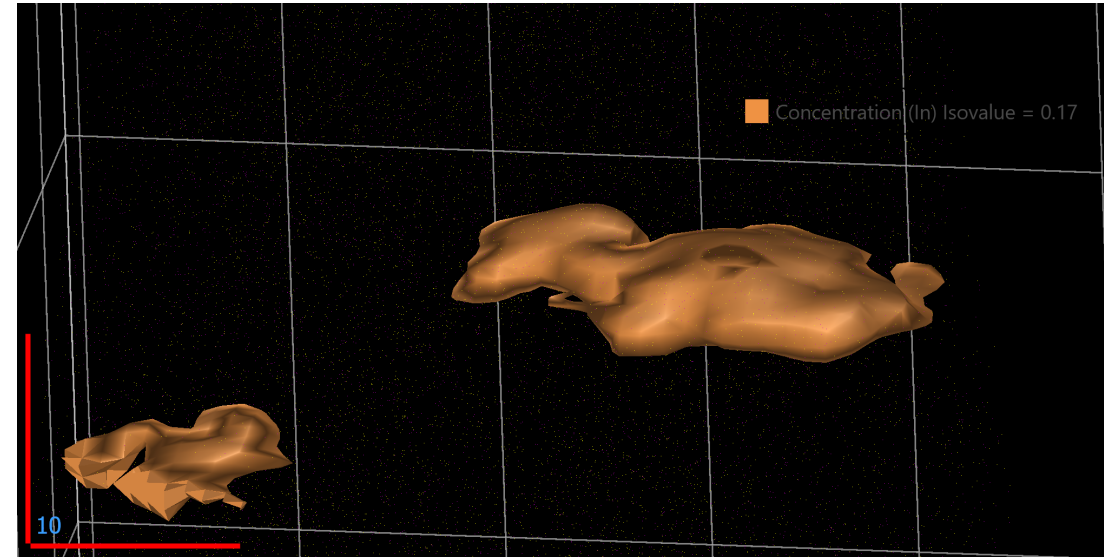


Isosurface - SKQD

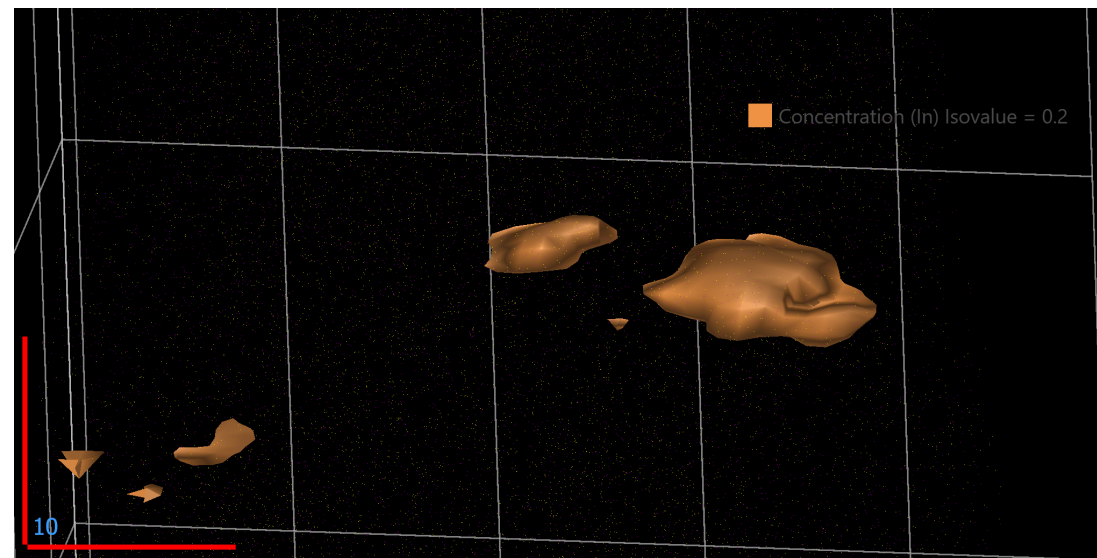
10%



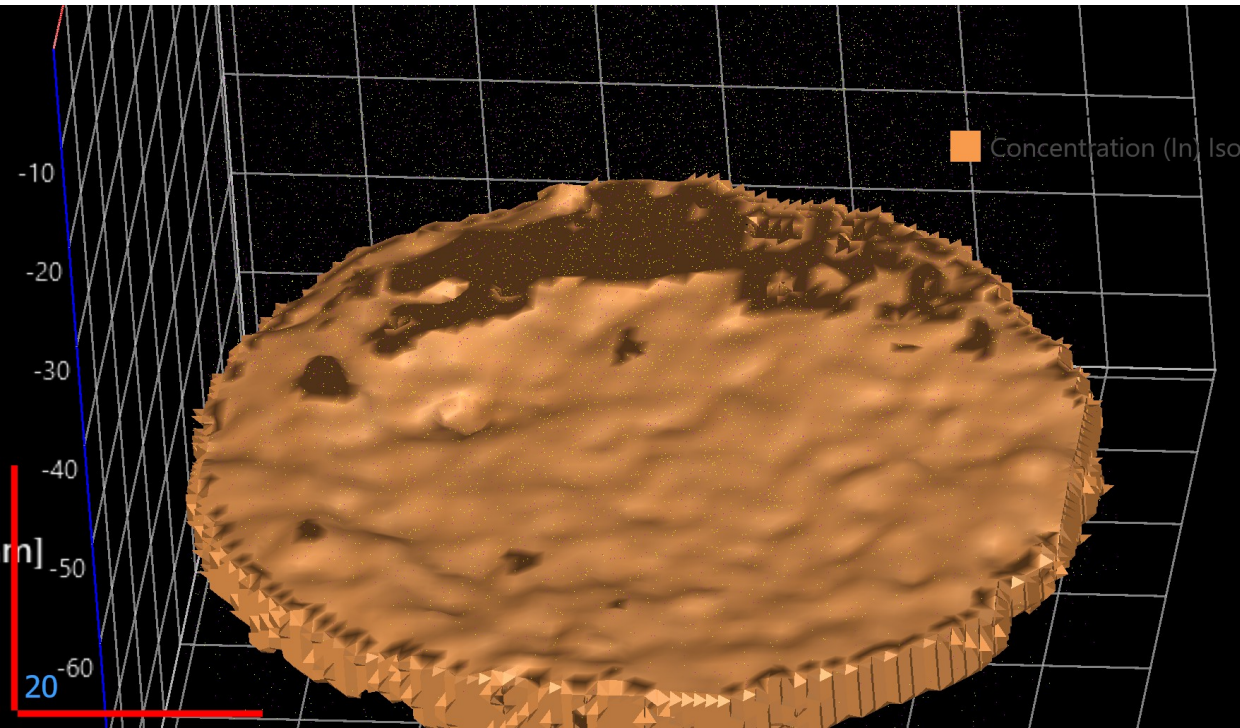
17%



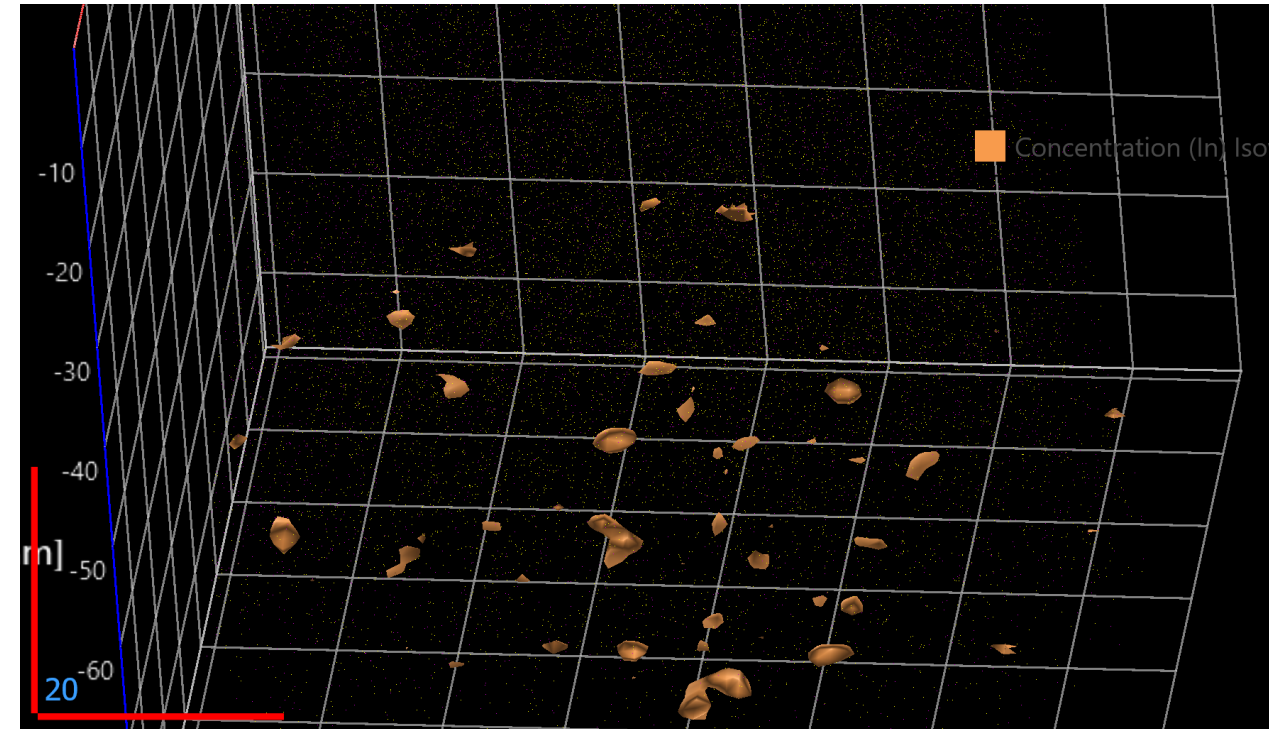
20%



Isosurface – c(4×4) SMLQD



6%



15%

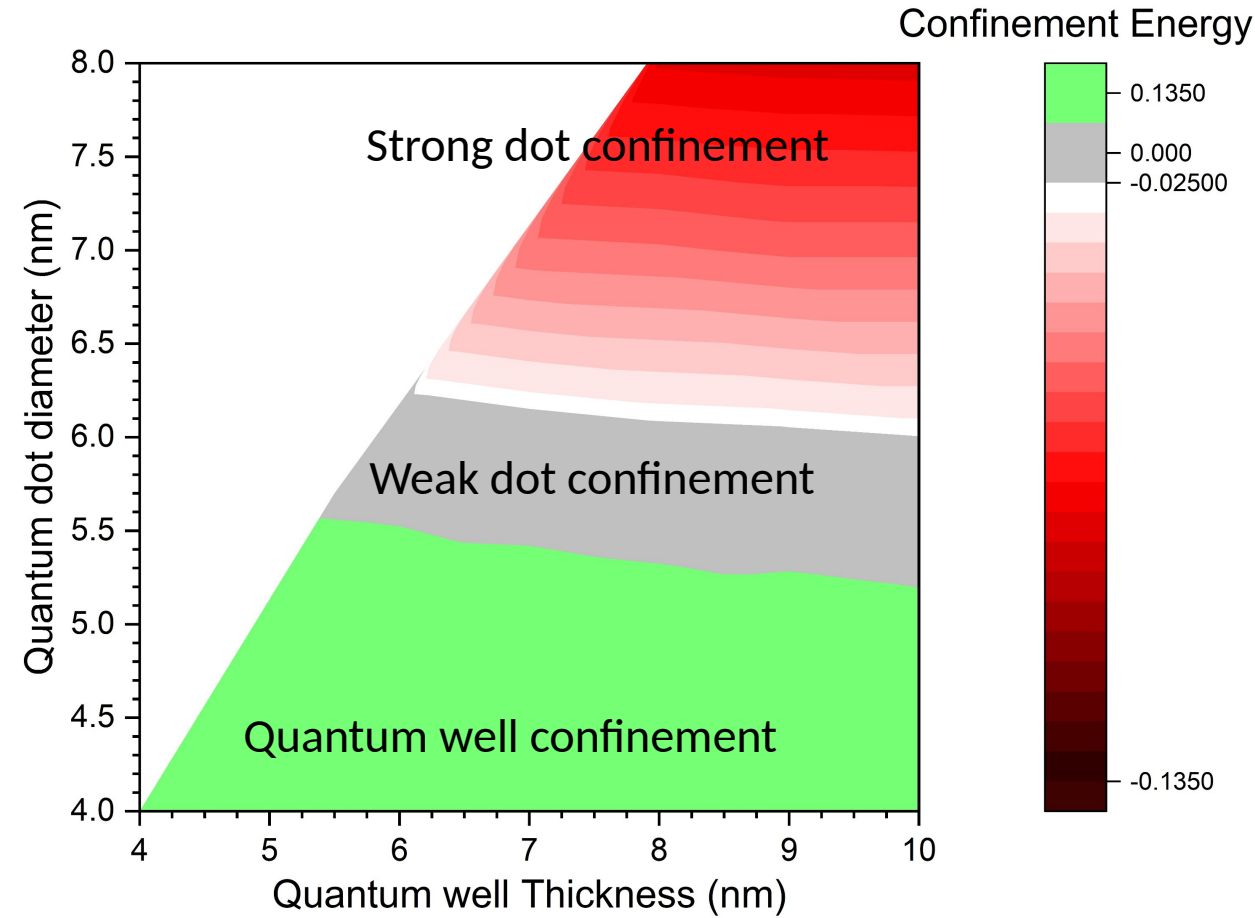
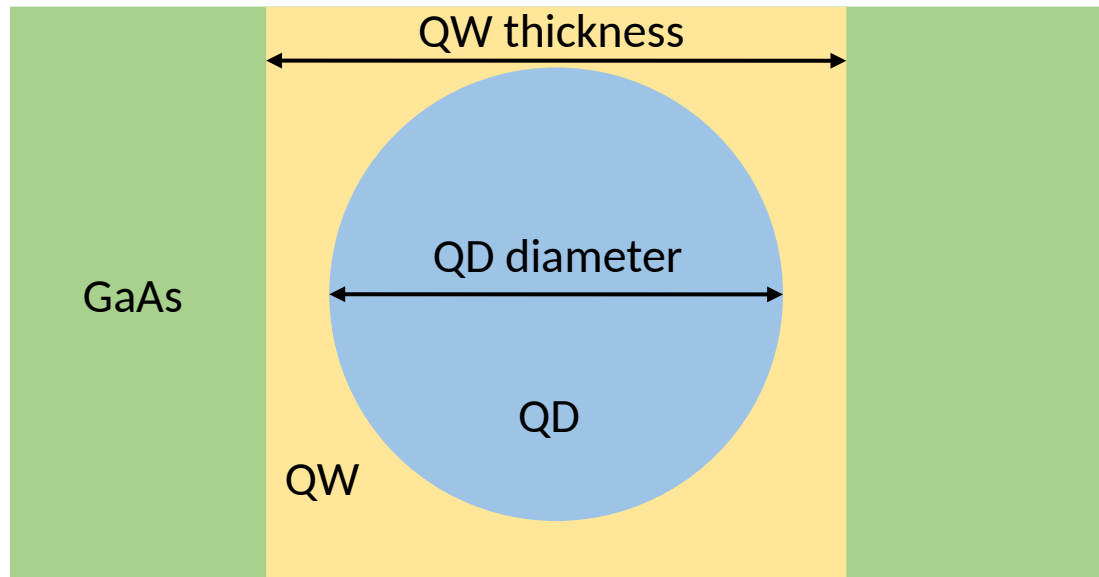
Cluster analysis

Cluster parameters	
d-max (nm)	0.7
Order (ions)	10
N-min (ions)	200
L (nm)	0.7
d-erosion (nm)	0.4

	In %	Extent x (nm)	Extent y (nm)	Extent z (nm)	Volume (nm ³)
Matrix	7.5	-	-	-	-
Cluster 1	17.9	6.1	3.0	2.5	189
Cluster 2	18.7	9.4	6.5	2.2	551
Cluster 3	17.7	4.0	4.5	2.0	155
Cluster 4	18.1	2.9	5.1	2.4	150
Cluster 5	18.3	3.6	3.9	2.2	130
Cluster 6	18.9	4.4	2.4	2.5	113
Cluster 7	18.3	2.9	3.7	1.8	81
Cluster 8	16.6	5.3	3.5	1.8	139
Cluster 9	18.0	2.8	4.3	2.6	130
Cluster 10	19.0	4.7	4.9	2.4	232
Cluster 11	17.2	6.7	4.5	2.1	262

c(4×4) SMLQD

Cluster analysis



Final remarks

- The only technique that provides 3D compositional information with nano or sub nanometer resolution.
- FIB/SEM to make a cone-shaped sample.
- Sample is evaporated, collected, and reconstructed.
- Analysis: stoichiometry, cluster existence (nearest neighbor), concentration as a function of distance (radial distribution), degree of clusterization (correlation function), 3D shapes above a threshold concentration (isosurface), cluster identification.
- APT as simulation input.
- Understanding nanostructures and nanodevices.