An Autonomous Platform for ML-guided SAXS/SANS on Liquid Formulations

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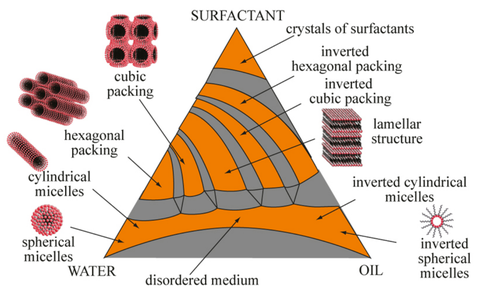
Industrial Soft Materials are Multicomponent

Soft materials manufacturing is enabled by navigation of phase diagrams with many components

- Formulations with >10 components common among nSoft members
- Number of phases in >10-dimensional space can be far larger (or smaller)



https://eng.thesaurus.rusnano.com/wiki/article513

Ingredient	
Amyl Butyrate – 10%	Linalol
Borneol Cryst	Linalyl Acetate
Butyl Acetate – 1%	Linalyl Oxide
Camphene – 10%	Myrcene – 10%
Caryophyllene	Ocimene
Coumarin – 10%	Pinene alpha
DPG	Pinene beta – 10%
Eucalyptol	Terpineol
Geranyl Acetate	Terpinolene
Jasminone B – 10%	Vetiver Haiti – 10%
Limonene	

Components of Typical Lavender 'Accord' Fragrance Blend

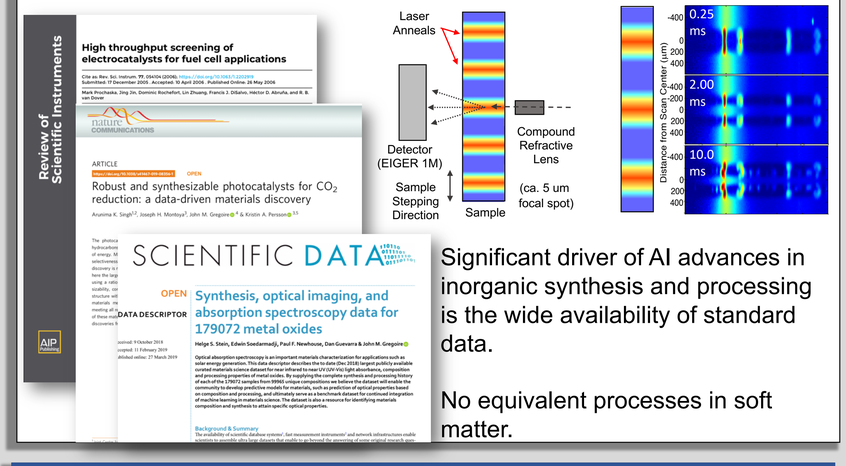
Need to maintain a preferred place in phase space as formulation varies to meet product needs

- A preferred phase is often determined in discovery phase
- Mapping the process window for multicomponent systems requires exponentially increasing number of experiments

Example Formulation Application Spaces

Personal Care Products	**mRNA Vaccine Carriers**	**Biologic Drug Stabilization Systems**
Pigments	**Nanoparticle Solution Syntheses**	**Battery Electrolytes**
Lipid vesicles	**Concentrated Monoclonal Antibodies**	**Engineered Food Products (e.g. Plant-Based Meat)**

AI/ML Widely Used in Inorganic Materials



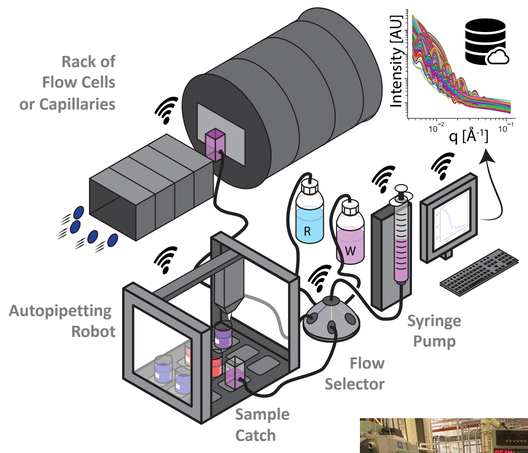
Significant driver of AI advances in inorganic synthesis and processing is the wide availability of standard data.

No equivalent processes in soft matter.

Project Goals

1. **Enable machine-guided, high throughput exploration of liquid formulations.**
2. **Generate high-quality datasets on soft material liquids.**
3. **Create a flexible sample environment for nSoft/NCNR user experiments.**
4. **Expand application space from soft matter into hybrid organic-inorganic functional materials.**

NistoRoboto: automated liquid handling



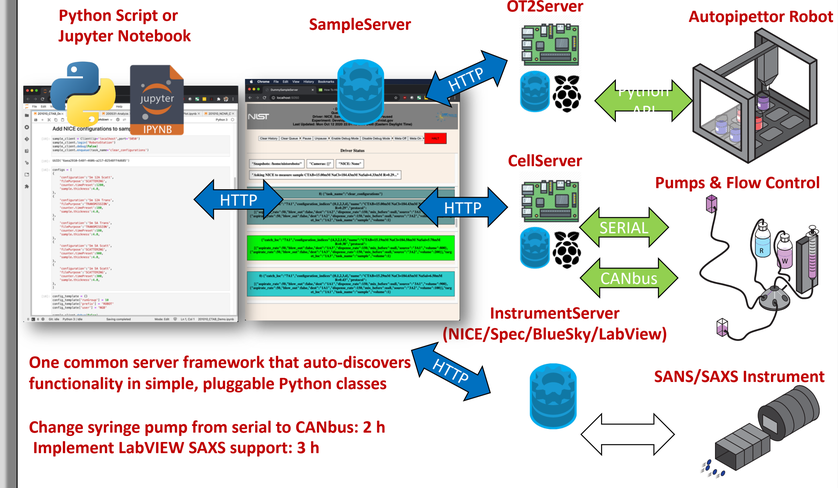
Flexible, standards-based, microservice-driven platform to integrate preparation, loading, and multimodal measurement on a single platform.

An IoT approach to instrument automation.

Integration w/ SANS instruments @ NCNR, SAXS instruments @ CHESS and MSED, UV-vis, optical imaging.

Open design allows rapid integration of new hardware.

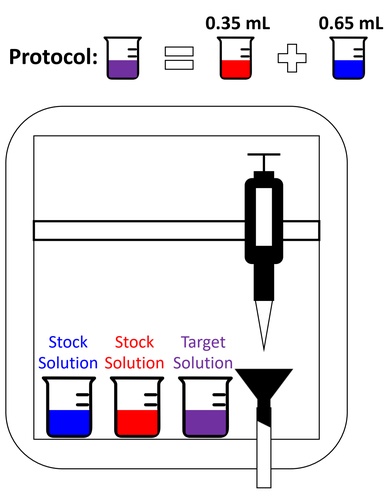
Python-based Microservice Software Backend



One common server framework that auto-discovers functionality in simple, pluggable Python classes

Change syringe pump from serial to CANbus: 2 h
Implement LabVIEW SAXS support: 3 h

Teaching Python Chemistry 101 and Mass Balances



Simplified Script Example

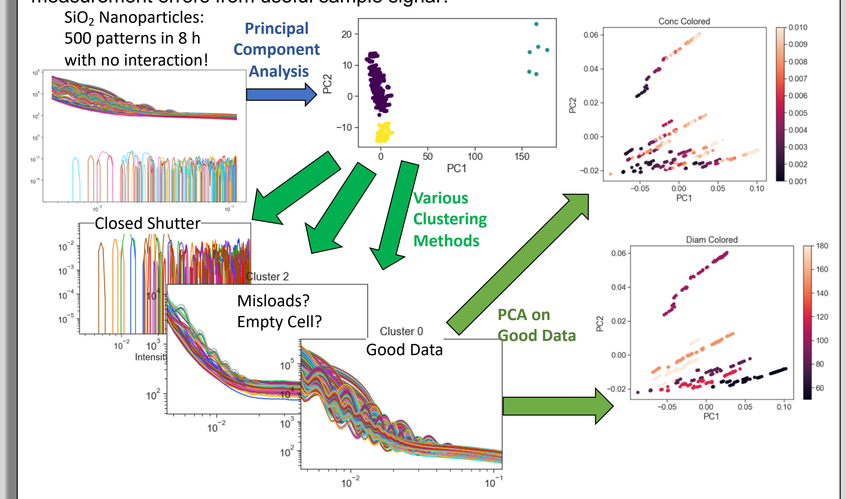
```
H2O  = Component('H2O',density=1.00)
D2O  = Component('D2O',density=1.11)
salt = Component('salt',mass=1.0)
SDS  = Component('SDS',mass=1.0)

target_solution = Mixture([H2O,D2O,SDS,salt])
target_solution.set_mass_fractions({
                                    'H2O':0.2,
                                    'D2O':0.75,
                                    'SDS':0.045,
                                    'salt':0.005
                                    })

deck = Deck() # pipettor deck abstraction
deck.add_stock(stock_D2O,'3A1')
deck.add_stock(stock_D2O,'3A2')
deck.add_stock(stock_salt,'6A1')
deck.add_stock(stock_SDS,'6A2')

deck.add_target(target_solution,'1A1')
deck.make_protocol(volume_cutoff=0.03)
deck.send_protocol()
```

Real Script for Surfactants

```
orig_stock_red = NistoRoboto.prep.Mixture.Mixture([D2O,CTAB,NaCl])
orig_stock_red['D2O'].mass = 55.7121*units.g
orig_stock_red['NaCl'].mass = 0.0060*units.g
orig_stock_red['CTAB'].mass = 0.3802*units.g

orig_stock_yellow = NistoRoboto.prep.Mixture.Mixture([D2O,CTAB,NaCl,NaSal])
orig_stock_yellow['D2O'].mass = 55.6629
orig_stock_yellow['NaCl'].mass = 0.0063
orig_stock_yellow['NaSal'].mass = 0.0837
orig_stock_yellow['CTAB'].mass = 0.4055

orig_stock_pink = NistoRoboto.prep.Mixture.Mixture([D2O,NaCl])
orig_stock_pink['D2O'].mass = 55.4177
orig_stock_pink['NaCl'].mass = 0.0339

[['CTAB=15.00mM NaCl=184.43mM NaSal=4.33mM R=0.29',
  [<PipetteAction Vol:600.000 3A1—>1D5>,
   <PipetteAction Vol:400.000 3A2—>1D5>],
  '1D5'],
 ['CTAB=15.19mM NaCl=184.58mM NaSal=5.78mM R=0.38',
  [<PipetteAction Vol:800.000 3A1—>1D4>,
   <PipetteAction Vol:200.000 3A2—>1D4>],
  '1D4'],
 ['CTAB=15.29mM NaCl=184.65mM NaSal=6.50mM R=0.43',
  [<PipetteAction Vol:900.000 3A1—>1D6>,
   <PipetteAction Vol:100.000 3A2—>1D6>],
  '1D6']]
```

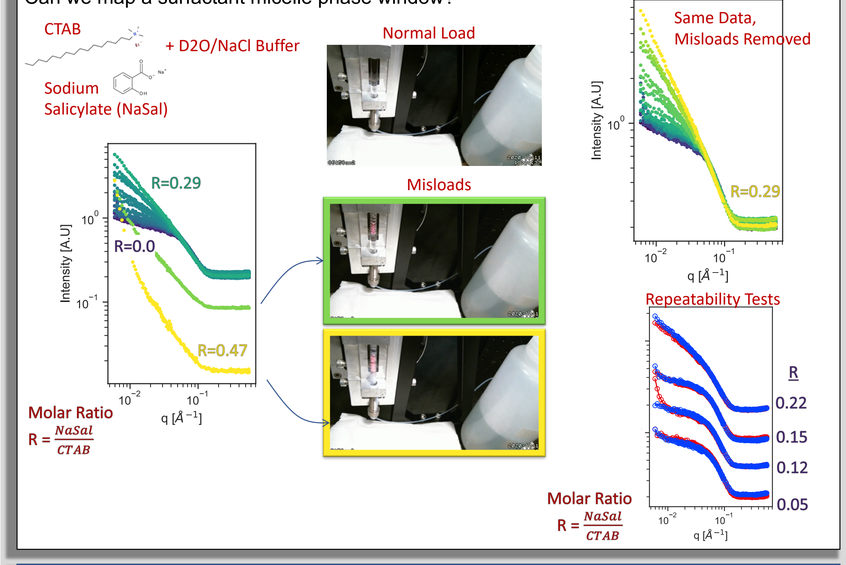
Application: Detection of Measurement Errors

Using a nanoparticle reference dataset, can we use unsupervised learning to differentiate measurement errors from useful sample signal?



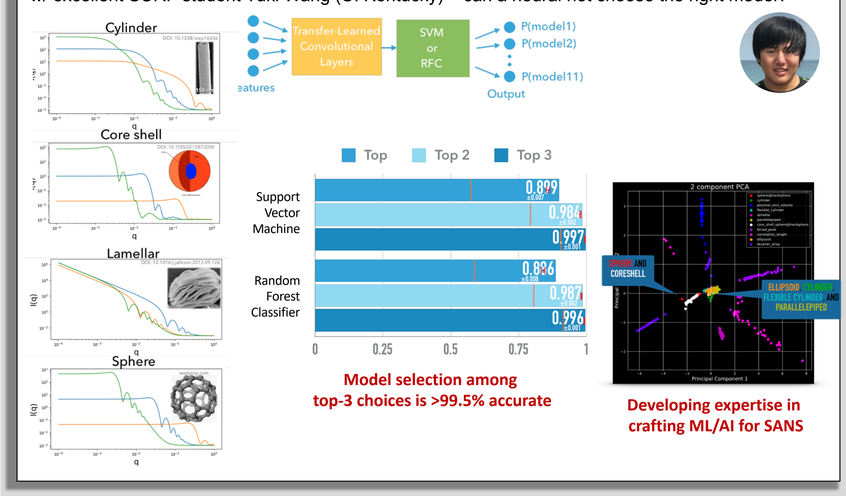
Application: Surfactant Micelle Extension

Can we map a surfactant micelle phase window?



Application: Neural Nets for Scattering Data

w/ excellent SURF student Yuki Wang (U. Kentucky) – can a neural net choose the right model?



Acknowledgments

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