The mathematics of finding atoms in nanoparticles

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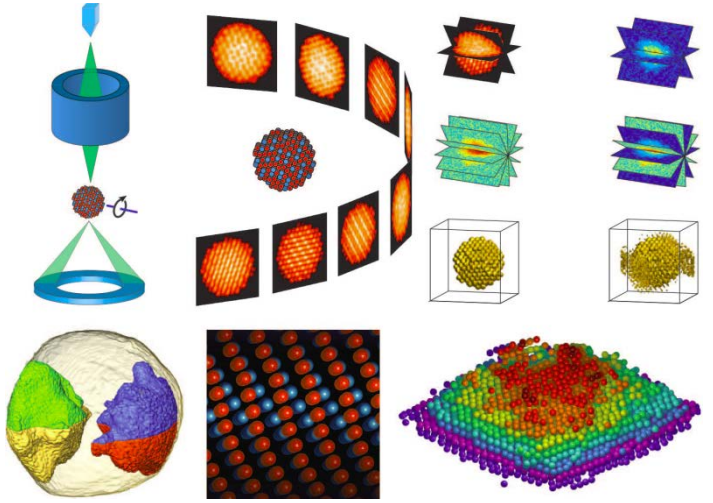
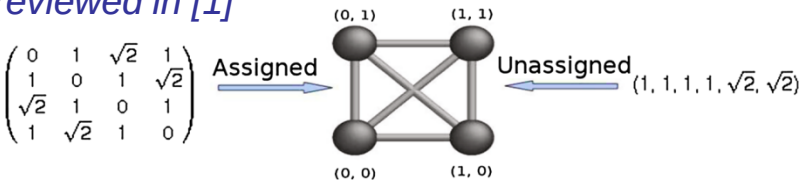
Columbia University **DMR-1534910**

- When atoms arrange themselves in crystals we have great tools for finding them: x-ray crystallography
- In nanostructures the atoms are much harder to find. But find them we must!
- Essential issues are
  - loss of signal in the experiments
  - loss of information in those signals
  - increased complexity of the structural solutions.
- We are addressing this three pronged attack by developing advanced mathematical, computational and data analytic approaches as part of our DMREF project.
  - The problem, and recent developments, have ben reviewed [1].
  - A sub-field of Graph Theory, Distance Geometry, has been explored to aid in the solution of nanostructure reconstructions from ensembles of particles [2].



Examples of different Nanostructure problems reviewed in [1]



A new sub-problem in graph theory, the ***Unassigned Distance Geometry Problem*** *has been defined that allows the use of powerful results from graph theory such as the concept of rigidity percolation to make nanostructure reconstruction algorithms more robust [2]*

[1] J. Miao, J., Ercius, P. & Billinge, S. J. L. *Atomic electron tomography: 3D structures without crystals*. Science **353,** aaf2157 (2016).

[2] S. J. L. Billinge, Duxbury, P. M., Gonçalves, D. S., Lavor, C. & Mucherino, A. *Assigned and unassigned distance geometry: applications to biological molecules and nanostructures*. 4OR-Q J Oper Res*,* **14***,* 1 (2016).

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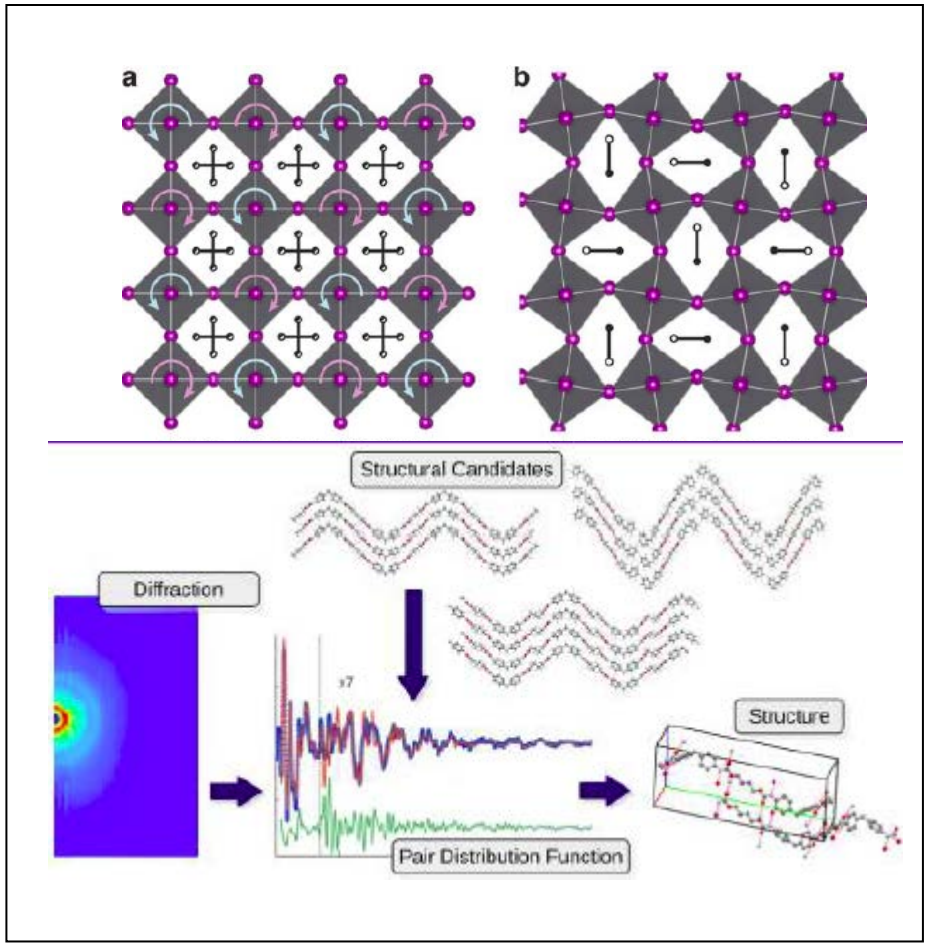

Nanotechnology will have an increasing impact on society as materials engineered at the nanoscale make their way into technologies such as monitors, solid-state lighting, photovoltaics, batteries and drug delivery

To realize this potential it is essential to be able to characterize atomic structure from these materials. The results of our DMREF will enable such technologies.

The impacts will be widespread because the methods we are developing are transformational and can be applied to many technologies, but to date in the DMREF we have applied them to

1. Emerging next generation low dimensional "Mxene" electronic materials [1]
2. Nanostructure of commercial polyurethane polymers has finally been revealed after decades of effort [2]
3. Secrets behind the performance of next generation materials for photovoltaics was revealed [3]

[1] B. Anasori, et. al, *Nanoscale Horiz.* **1**, 227-234 (2016).
[2] MW Terban, R Dabbous, AD. Debellis, E Pöselt and Simon J. L. Billinge, *Macromolecules* **49**, 7350-7358 (2016).
[3] AN Beecher, OE Semonin, JM Skelton, JM Frost, MW Terban, H Zhai, A Alatas, JS Owen, Aron Walsh and SJL Billinge *ACS Energy Lett.* **1**, 880–887 (2016).