

Center for Functional Nanomaterials



Center for Functional Nanomaterials SDCC TAB Stakeholders Meeting

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Sept. 6 2024
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The CFN is a dynamic, well-managed facility with high productivity & impact

From 2019–23, the CFN (Comprised of ~35 permanent scientific staff):

Increased the yearly number of users supported to 655

- The most ever for CFN in a year; 18% more than in 2018
- Supported 3,005 unique users in all; 15% more than prior 5-year period
- >90% of users are satisfied

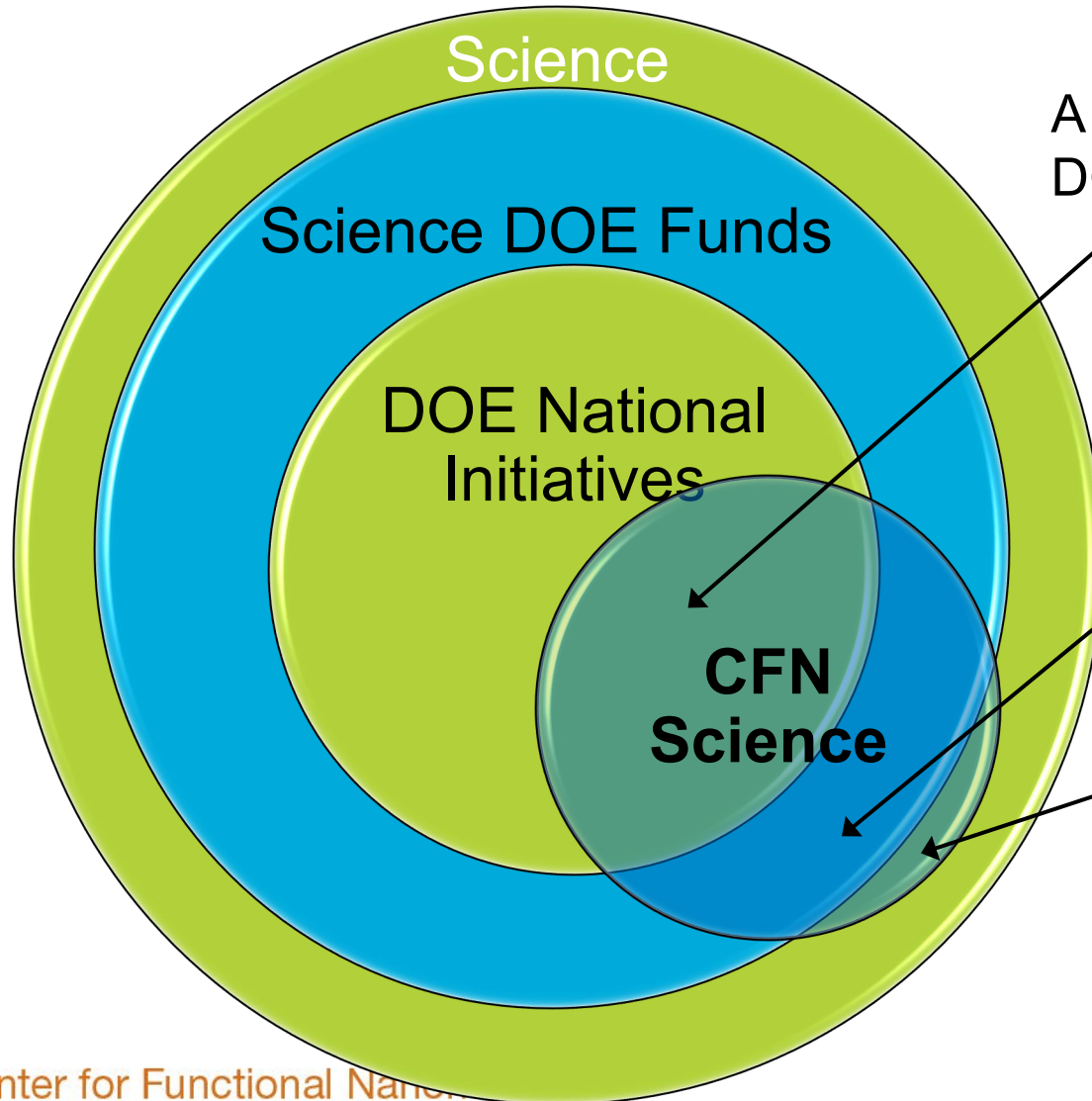
Supported 1,623 publications

- 13% more than prior five-year period
- Over half in high-impact journals (IF>7)

Efficiently managed operating resources and planned for the future

- Invested >\$20M in new instruments and upgrades

CFN supports a wide spectrum of research, including strong contributions to DOE & national science initiatives



A large fraction of research in the CFN is aligned with DOE & national science initiatives

- e.g., In 2022, 55% of pubs were **Clean Energy**
- (8% **QIS**; 9% **Microelectronics**)

CFN also supports DOE science projects that are not directly tied to national initiatives

Some CFN users are conducting research outside of core DOE interests. e.g.,

- **Art conservation:** MoMA and NYU
- **Bioscience:** (Dartmouth) “*Integrated Design of a Polypseudorotaxane-Based Sea Cucumber Mimic*”
- **Mars Mission Studies:** (St. Josephs) “*Studies on the effects of hypomagnetic field...*”

CFN supports a portfolio of facilities that integrate the full-cycle of materials research

CFN invested >\$20M in instrumentation and upgrades during 2019–23

Materials Synthesis & Characterization

Nanofabrication

Advanced Optical Spectroscopy & Microscopy

Electron Microscopy

Proximal Probes

Advanced UV & X-ray Probes

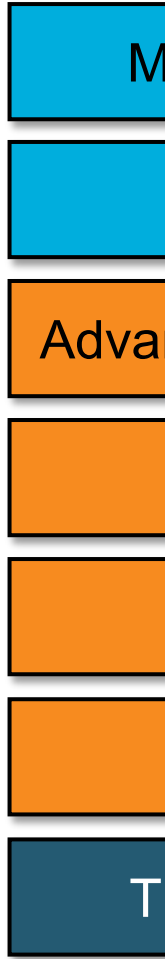
Theory, Computation, & Data Analytics



“Understanding” “Characterizing” “Making”

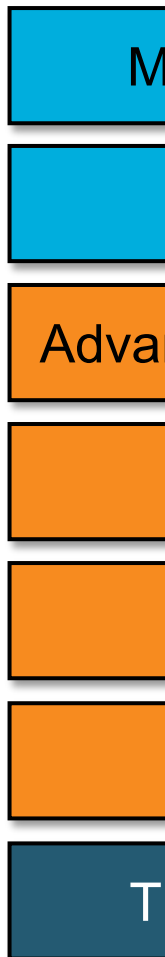
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“Understanding” “Characterizing” “Making”



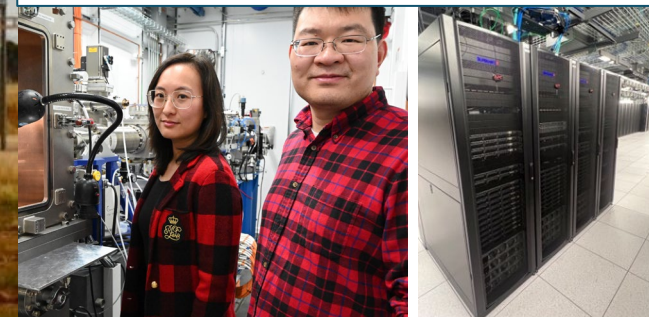
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“Understanding” “Characterizing” “Making”



Observations

- Individuals buying/maintaining equipment (data storage racks, GPU workstations)
- Staff are driven to make research progress, if there is no “clear path” they are compelled to go it alone.



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“Making”
“Characterizing”
“Understanding”

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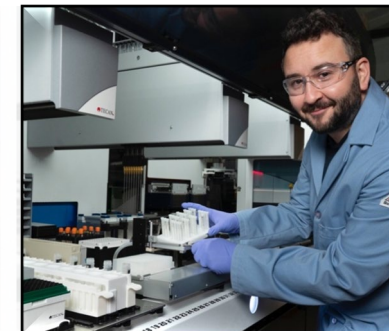
Proximal Probes

Advanced UV & X-ray Probes

Theory, Computation, & Data Analy



Quantum Material Press



Liquid Robot

Automated “synthesis by assembly” robotic systems

- Quantum Material Press (2D materials)
- Liquid Robot (DNA and biomolecule assembly)
- Autonomous experimentation platforms
- Potential to build relationships with SDCC:
 - Data storage
 - GPU workstations and/or alternatives

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“Making”
“Characterizing”
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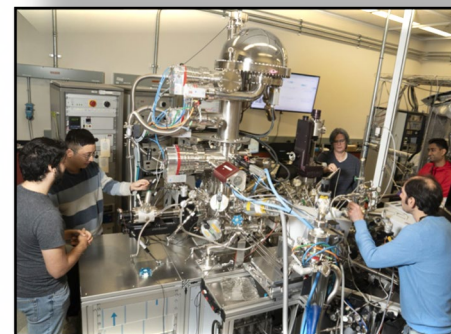
Proximal Probes

Advanced UV & X-ray Probes

Theory, Computation, & Data Analytics

In situ electron microscopy and surface science

- High-resolution ETEM
- Ambient pressure XPS and IR spectroscopy
- Multi-modal studies via compatible sample holders
- Potential to build relationships with SDCC:
 - Data streams (~3 GB/s → 50 GB/s (4D camera))
 - Data volumes (~100 TB/day)
 - Real-time data processing



AP-XPS



E-TEM



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“Understanding” “Characterizing” “Making”



Advanced UV & X-ray Probes

Theory, Computation, & Data Analytics

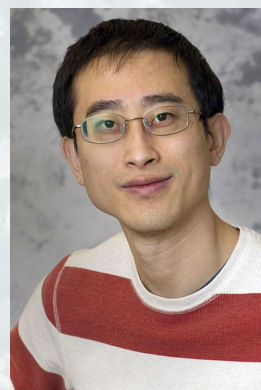
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Theory and Computation

- Stakeholder in ic2 (35 CPU + 8 GPU)
- Remix partition (54 nodes from ic1)
- CFN allocates computational resources to scientific “Users.”
 - Remote access for ~80 scientists, many from academia
 - ~80% Physics-based modeling, task computing suited to single high-memory nodes
- **MOU with SDCC**
- Potential to build relationship with SDCC:
 - Help compiling and optimizing scientific software (VASP)
 - Resource management (multiple queues on different hardware)
 - Awareness of resource utilization
 - Documentation (/scratch policy, contacts)
 - Future:
 - Heterogeneous resources (cloud and cluster)
 - Data infrastructure (generation, acquisition, storage, sharing)

Theory & Computation

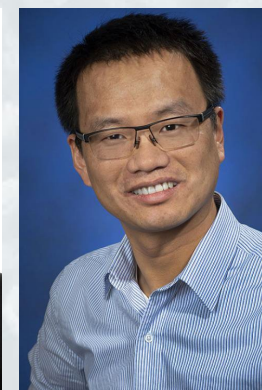
Sara E. Mason
Group Leader



Deyu
Lu



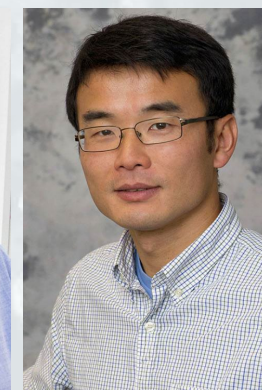
Sara
Mason



Xiaohui
Qu



Alexei
Tkachenko



Qin
Wu

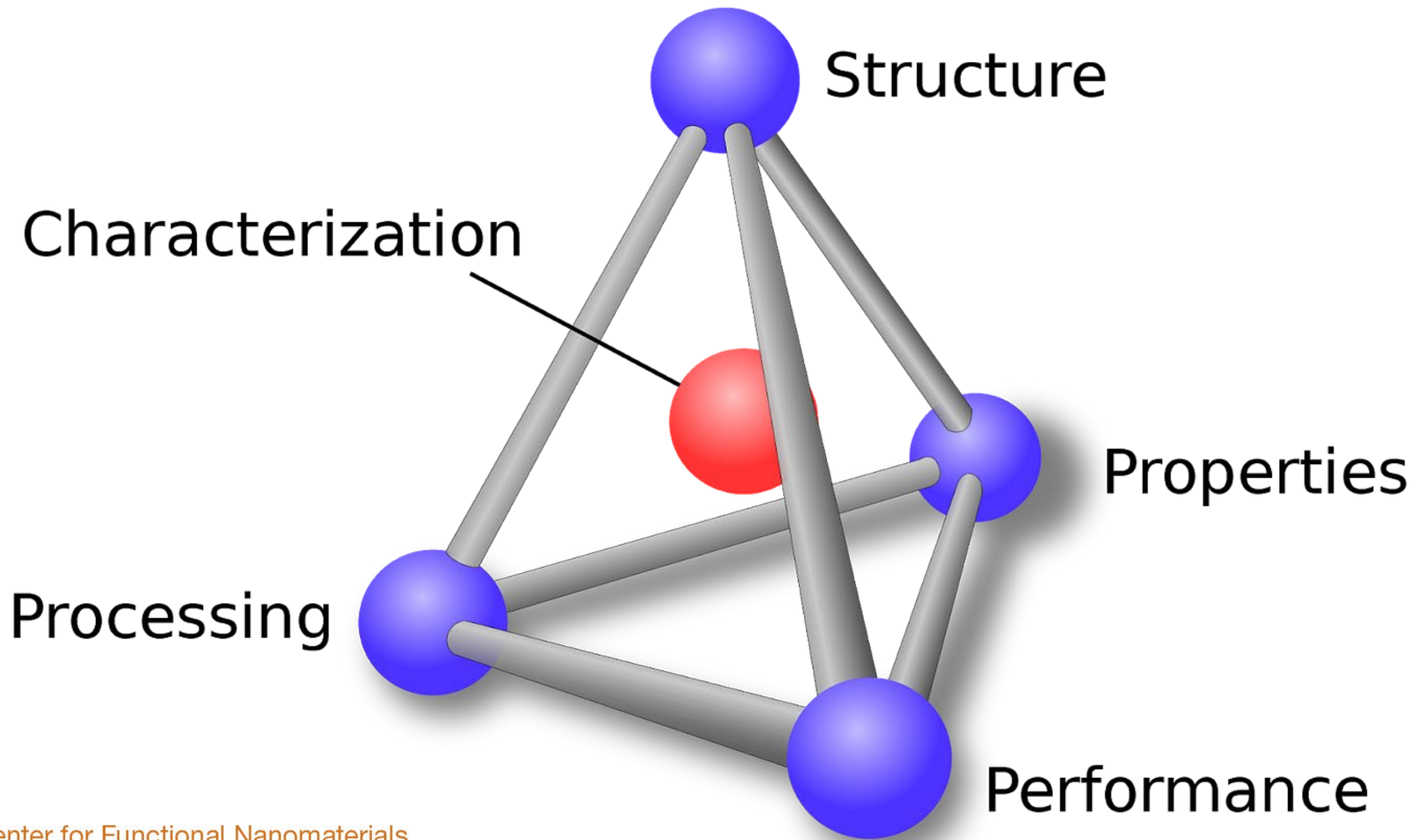
Theory & Computation: Expertise & Facilities



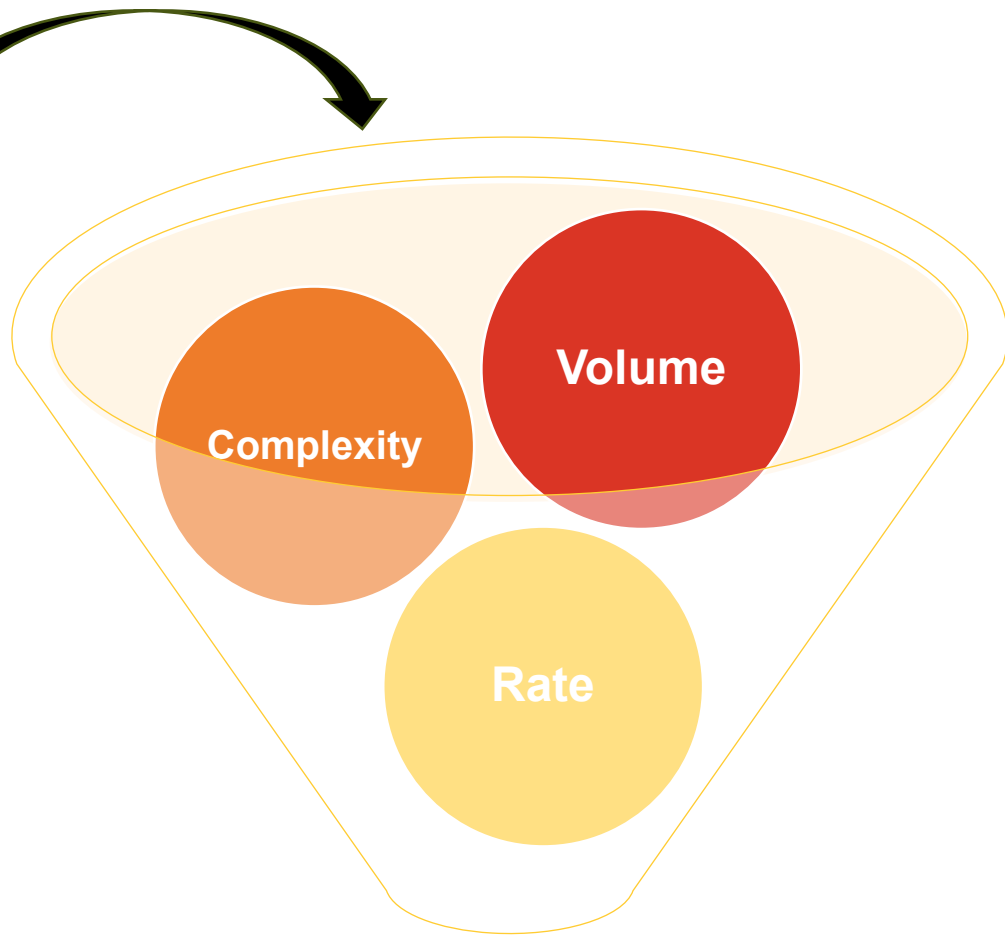
CFN Computing Facts:
FY 23: 22 M core-hours
FY 24: 18 + 17 = 35 M core-hours
 Consistent high rate of utilization

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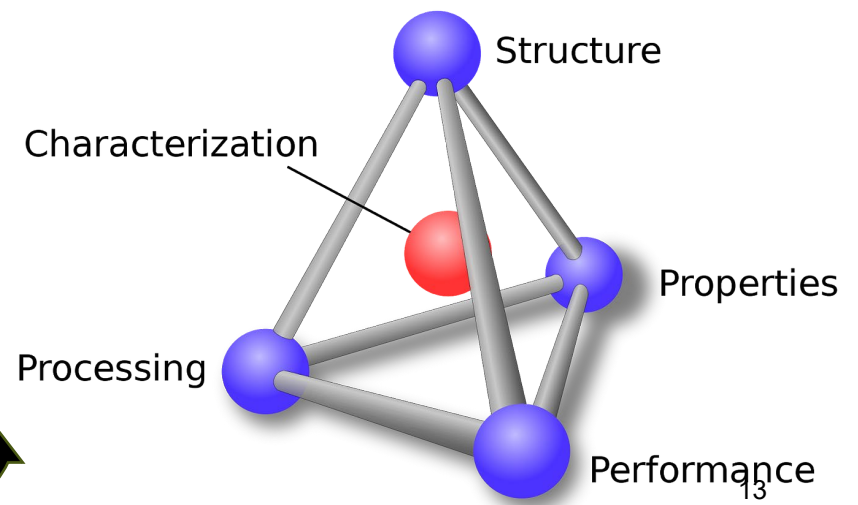




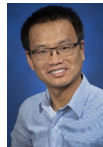
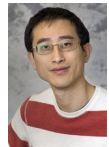
DATA



New AI/ML Tools



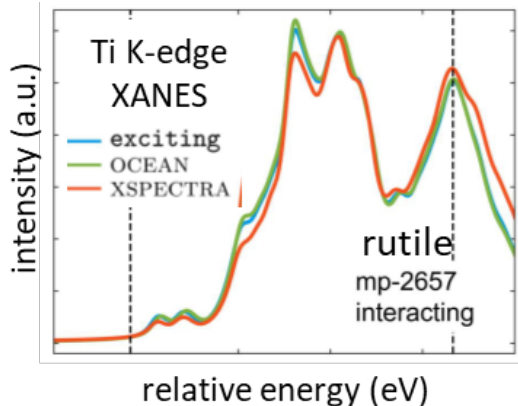
Cross-cutting AI/ML tools to accelerate nanomaterials discovery and characterization



Deyu Lu

Xiaohui Qu

Phys. Rev. Mat. 8 013801 2024



```
[1]: from lightshow import Database
    dat = Database.from_files(root="folder_name",
                             filename="POSCAR")

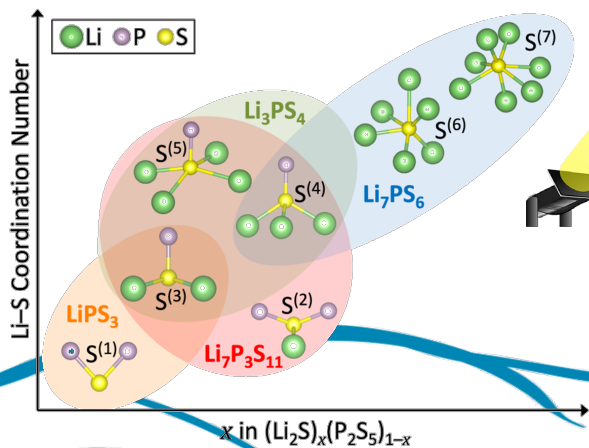
[2]: from lightshow import VASPParameters
    from lightshow.defaults import VASP_...
    params = VASPParameters(incar=VASP_..., edge="K",
                             potcar_directory=...)

[3]: dat.write("folder_name",
               absorbing_atoms="Ti",
               options=[params], ...)
```

Future Work:
Practical Approach to Finite T XANES

Scientific Data 10 349 2023

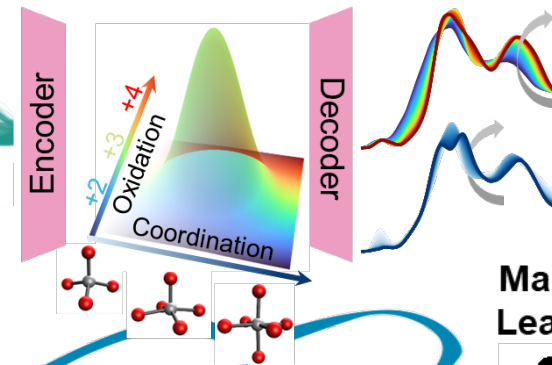
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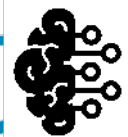
Workflow



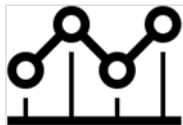
Phys. Rev. Mat. 7 053802 2023



Machine Learning



Benchmark



Poster

Database



End