Oak Ridge National Laboratory

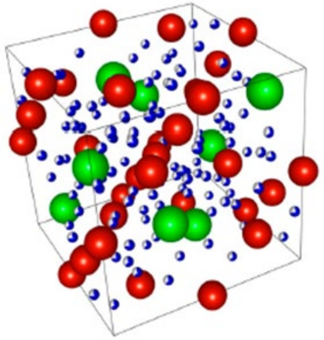
Atomistic modeling and machine learning for neutron scattering data analysis

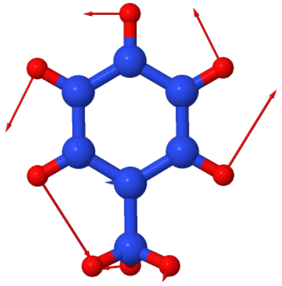
Yongqiang (YQ) Cheng

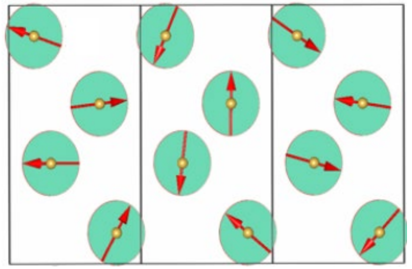
Spectroscopy Section
Neutron Scattering Division
Oak Ridge National Laboratory

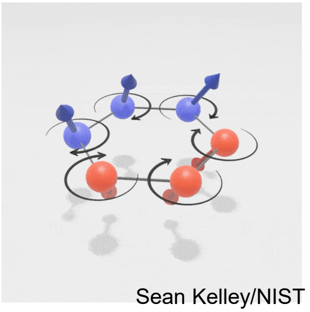
Atomistic modeling in neutron scattering

- Essential role in neutron data analysis and interpretation





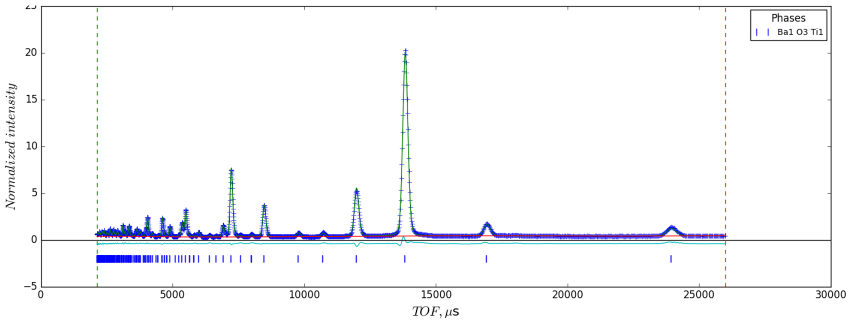


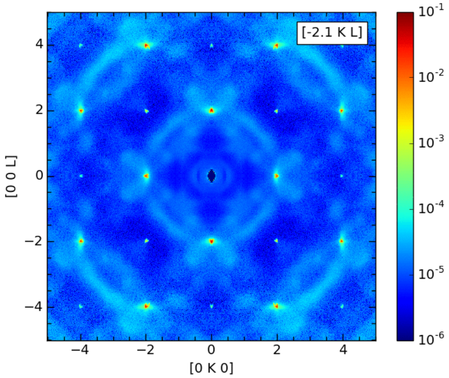


Jmol

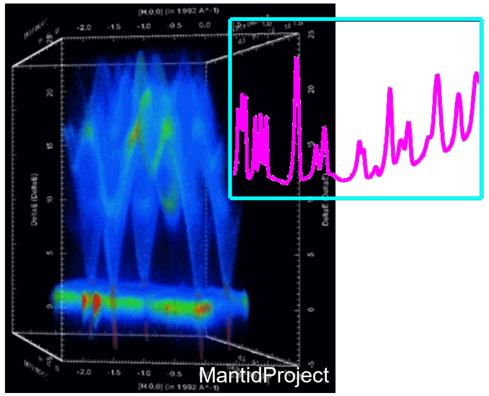
Atomic structure | Vibrational dynamics | Magnetic structure | Spin dynamics

Diffraction | Diffuse scattering | Spectroscopy





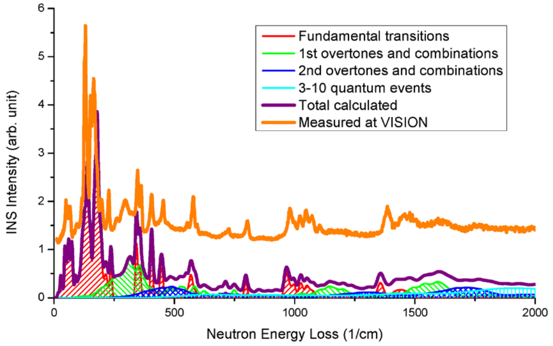
Yaohua Liu

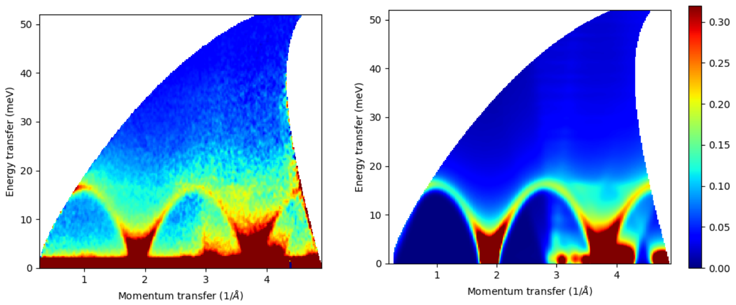


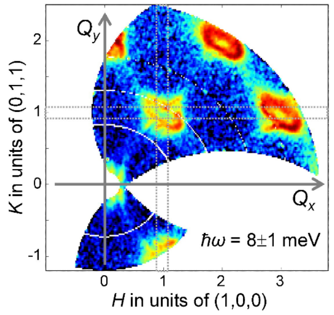
Bridging theory and INS experiments

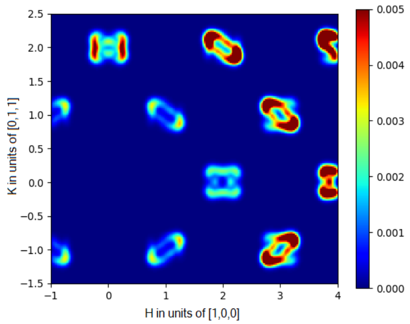
Common atomistic modeling tools

OCLIMAX



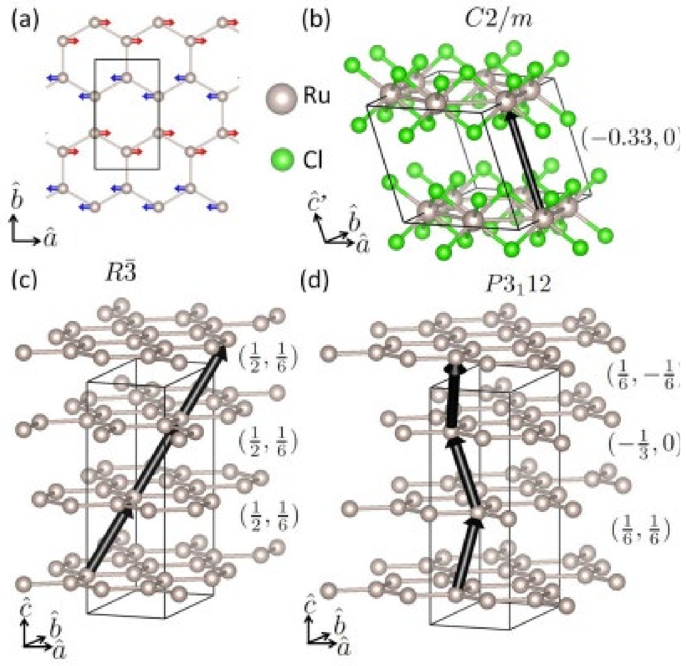


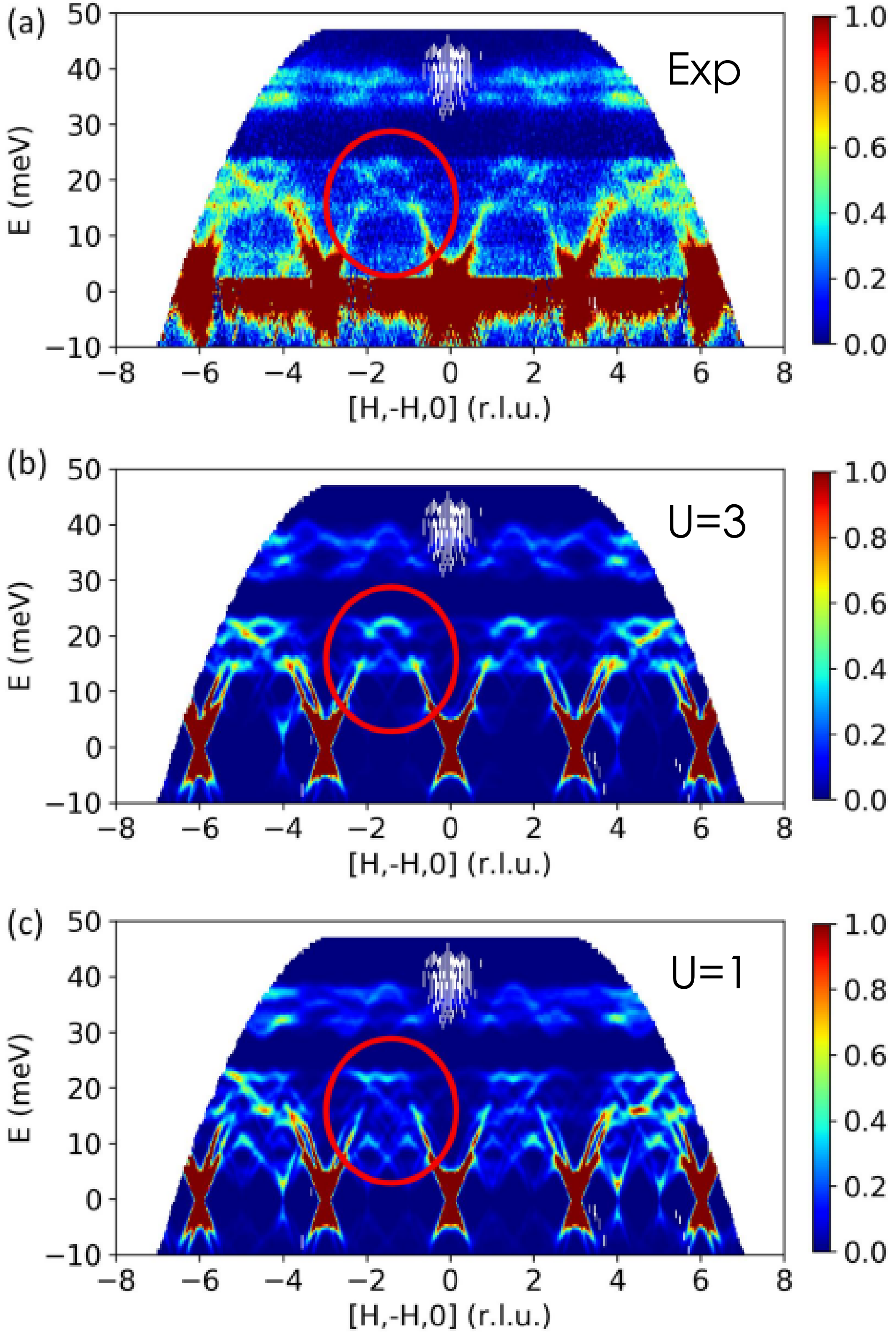


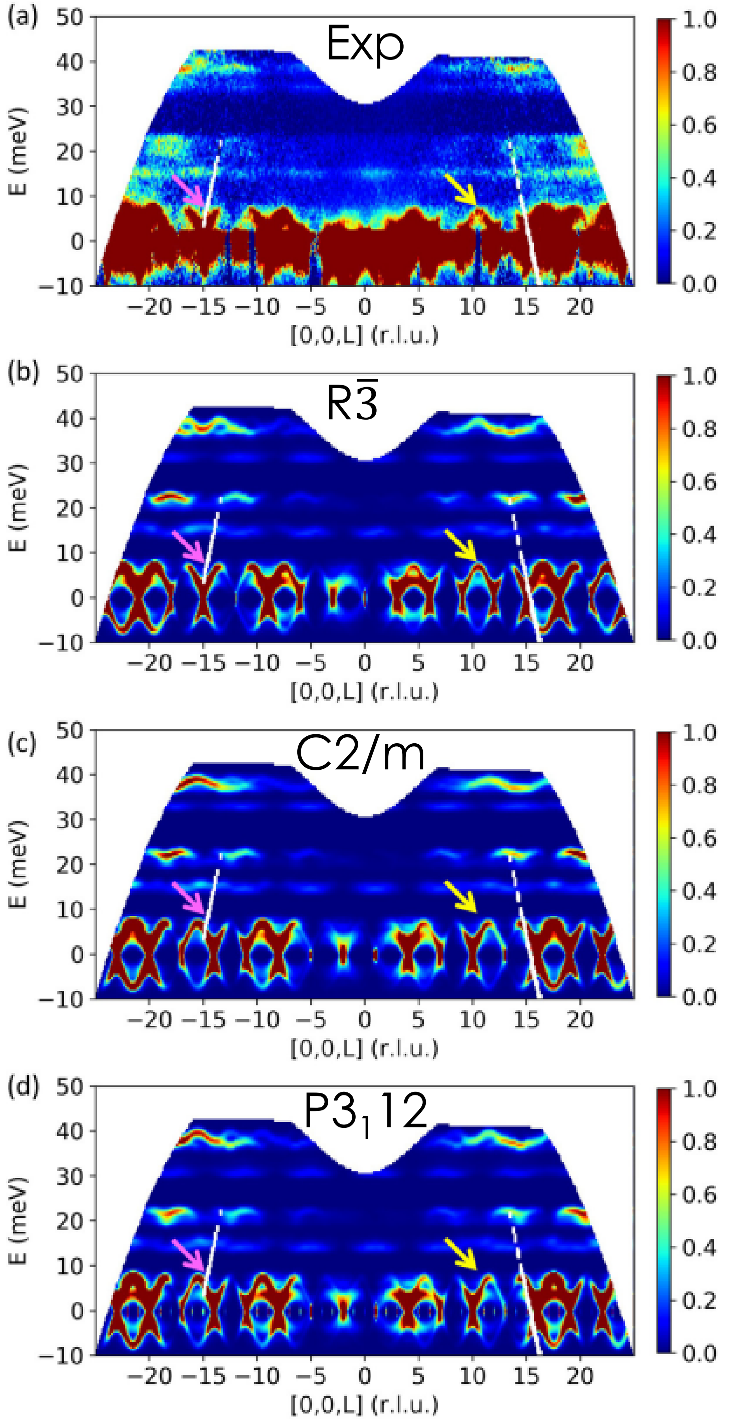


VISION, CNCS, HYSPEC, SEQUOIA, ARCS and many other neutron spectrometers.

Single crystal $RuCl_3$







S. Mu et al. Phys. Rev. Res., **4**, 013067 (2022)

Two grand challenges

- The model is not good enough for the science
  - Time and/or length scale limitations
  - Accuracy and efficiency trade-off

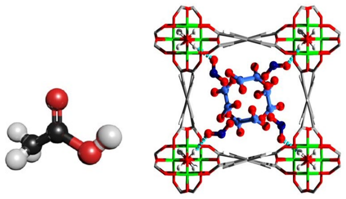
How much we can learn

- The analysis is not easy enough for the users
  - Computing resources
  - Learning curve

How many people can use it

How to predict neutron scattering features from an atomistic model?

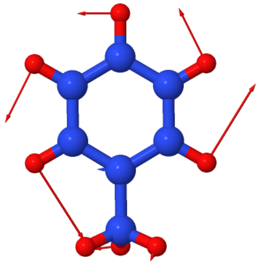
❖ What dictates the (nonmagnetic) features we see in a neutron scattering experiment (ideally)?



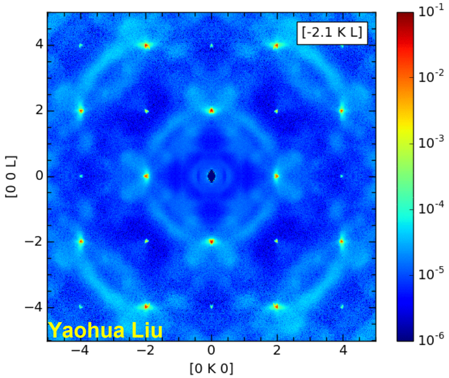
Atomic coordinates

$\{\ldots, E_i, \ldots\}$
$\{\ldots, f_{xi}, f_{yi}, f_{zi}, \ldots\}$

Atomic level energies and forces



Structure and dynamics



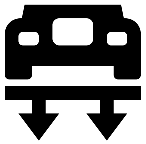
Neutron scattering features

❖ Given a structure, how to obtain the energies and forces (easily/quickly and accurately)?

✓ Traditional approach based on density functional theory (DFT)

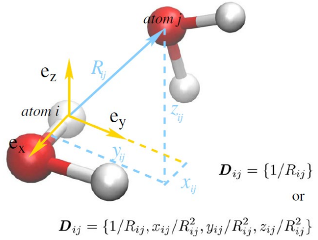
Accurate but slow/small

or classical force-fields

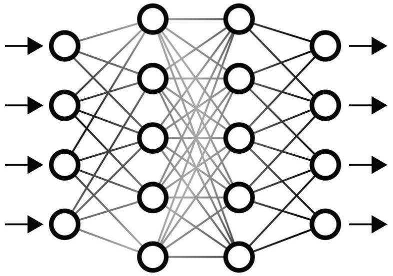


Fast/large but crude

✓ Machine learning force field (MLFF)



Embedding



Hidden layers

$\{\ldots, E_i, \ldots\}$
$\{\ldots, f_{xi}, f_{yi}, f_{zi}, \ldots\}$

Predicted energies and forces

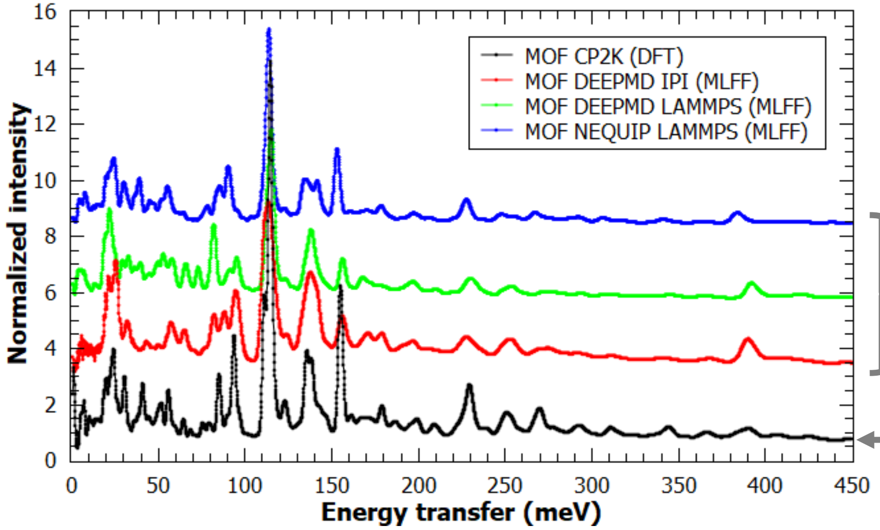
Fast/large with near DFT accuracy

Development and application of MLFFs in neutron scattering

Task:	DFT calculations to generate training datasets	Training of MLFFs	Atomistic modeling with MLFFs	Neutron scattering simulation	Analysis, visualization, and interpretation
Software:	VASP/CP2K/etc.	DeePMD etc.	LAMMPS etc.	OCLIMAX	Mantid/Dave/etc.
Hardware:	CADES/HPC	DGX	CADES/HPC/DGX Analysis/PC	Analysis/PC	Analysis/PC

DeepMD: Zhang et al. Phys. Rev. Lett. 120, 143001 (2018)
NequIP: Batzner et al. https://arxiv.org/abs/2101.03164 (2021)

✓ Simulation of vibration and INS spectra of complex materials



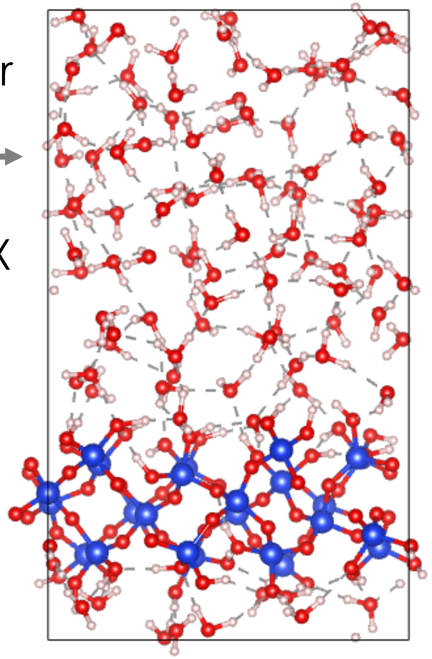
MLFF: Minutes on PC

DFT: Days on CADES

✓ Simulation of diffusion and QENS in heterogeneous systems

DFT: 1,000 steps per day on CADES

MLFF: 10,000 steps per minute on DGX

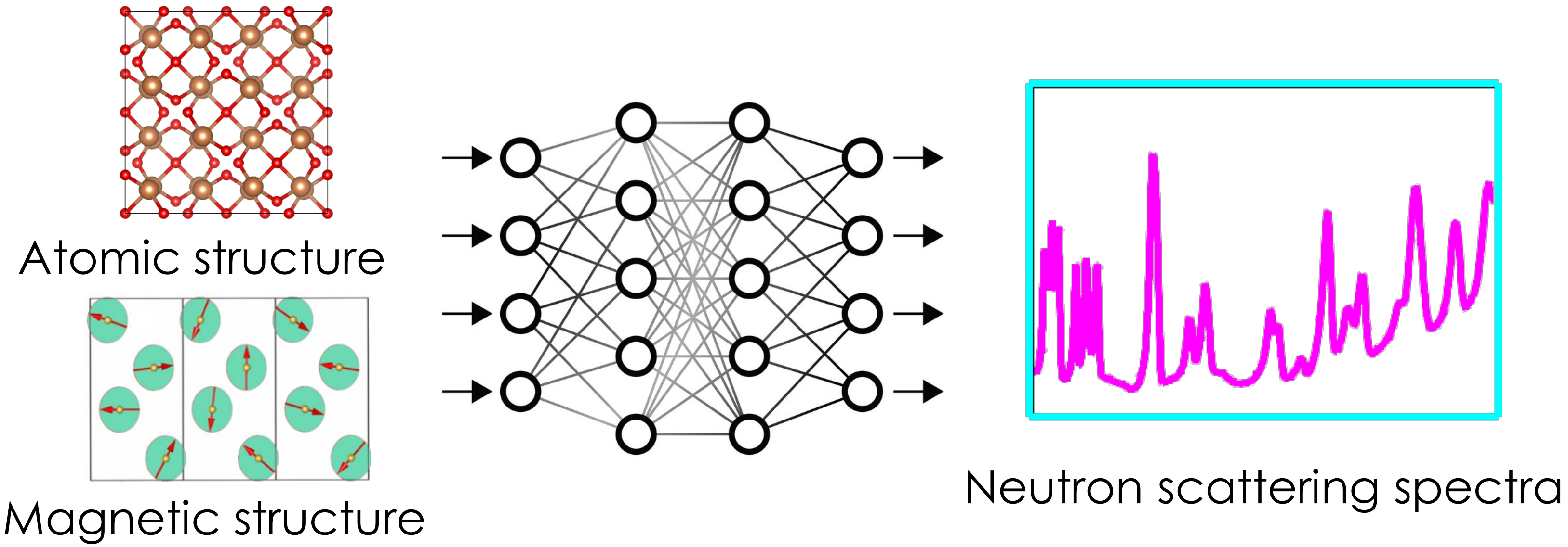


10,000 speedup and linear scaling with size, while inheriting spectroscopic accuracy from DFT

Opportunities

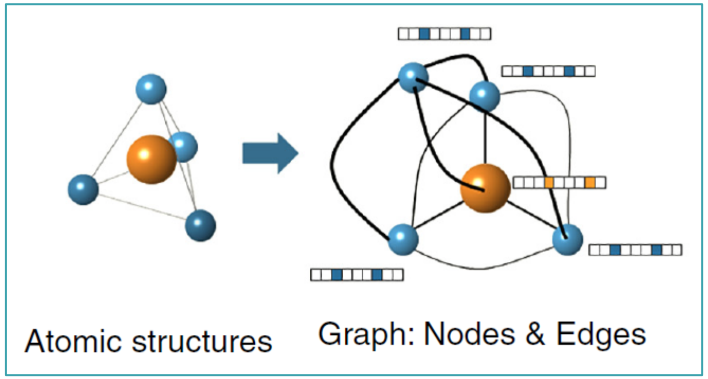
- Disordered/high-entropy materials
- Defects, surface, interface, domain boundaries
- Diffuse scattering (structural and thermal)

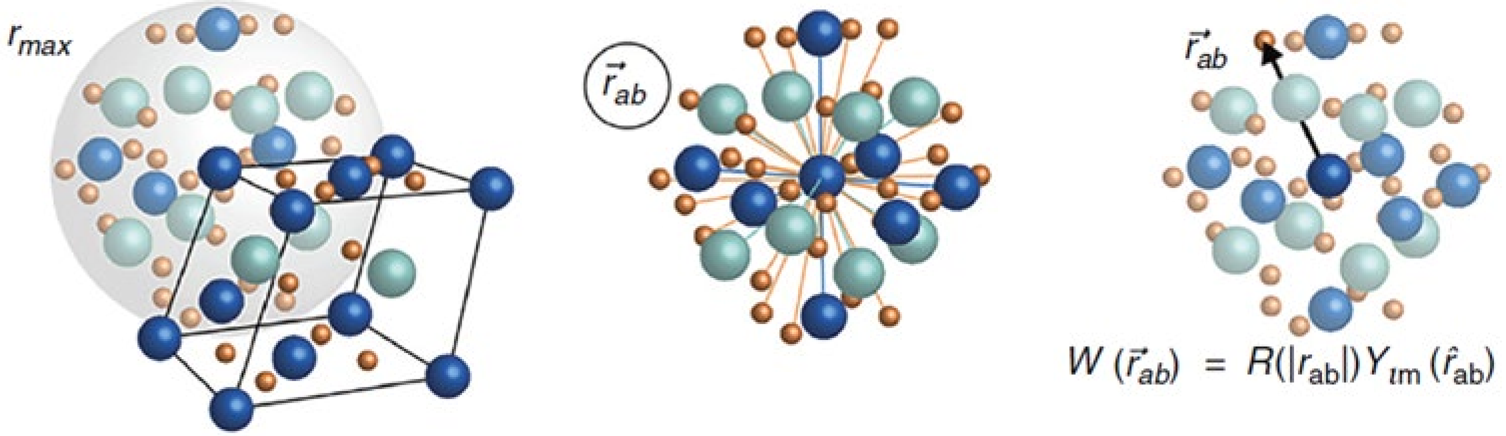
To tackle challenge 2: Neural networks connecting structure and neutron scattering data



Representation of structure

- Euclidean neural network (e3nn)





https://e3nn.org/
https://github.com/zhantaochen/phononDoS_tutorial

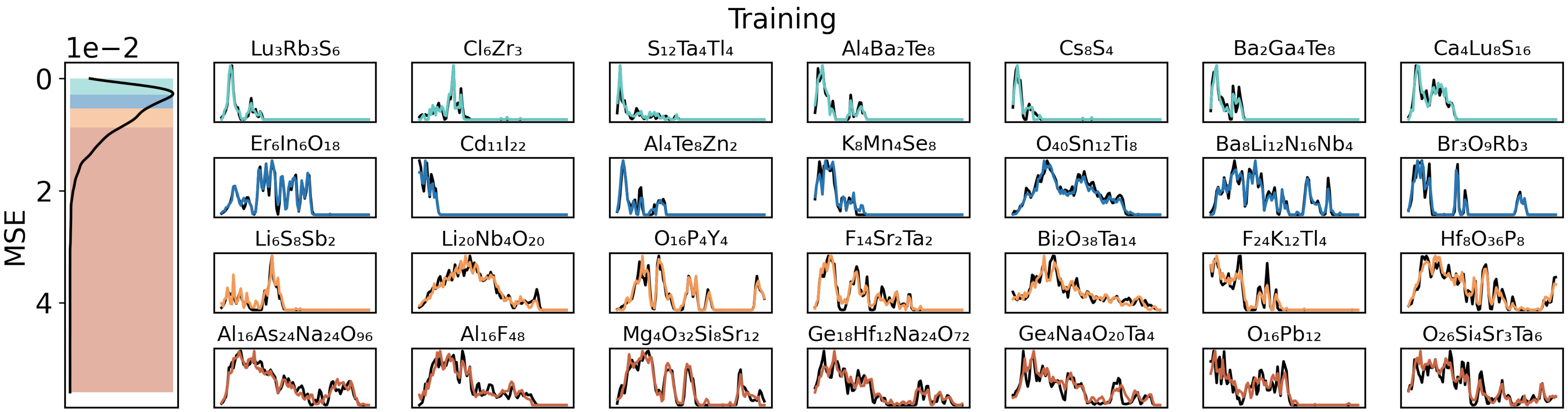
Equivariant neural network for 3D translation, rotation, inversion

In collaboration with Mingda Li and Tess Smidt at MIT

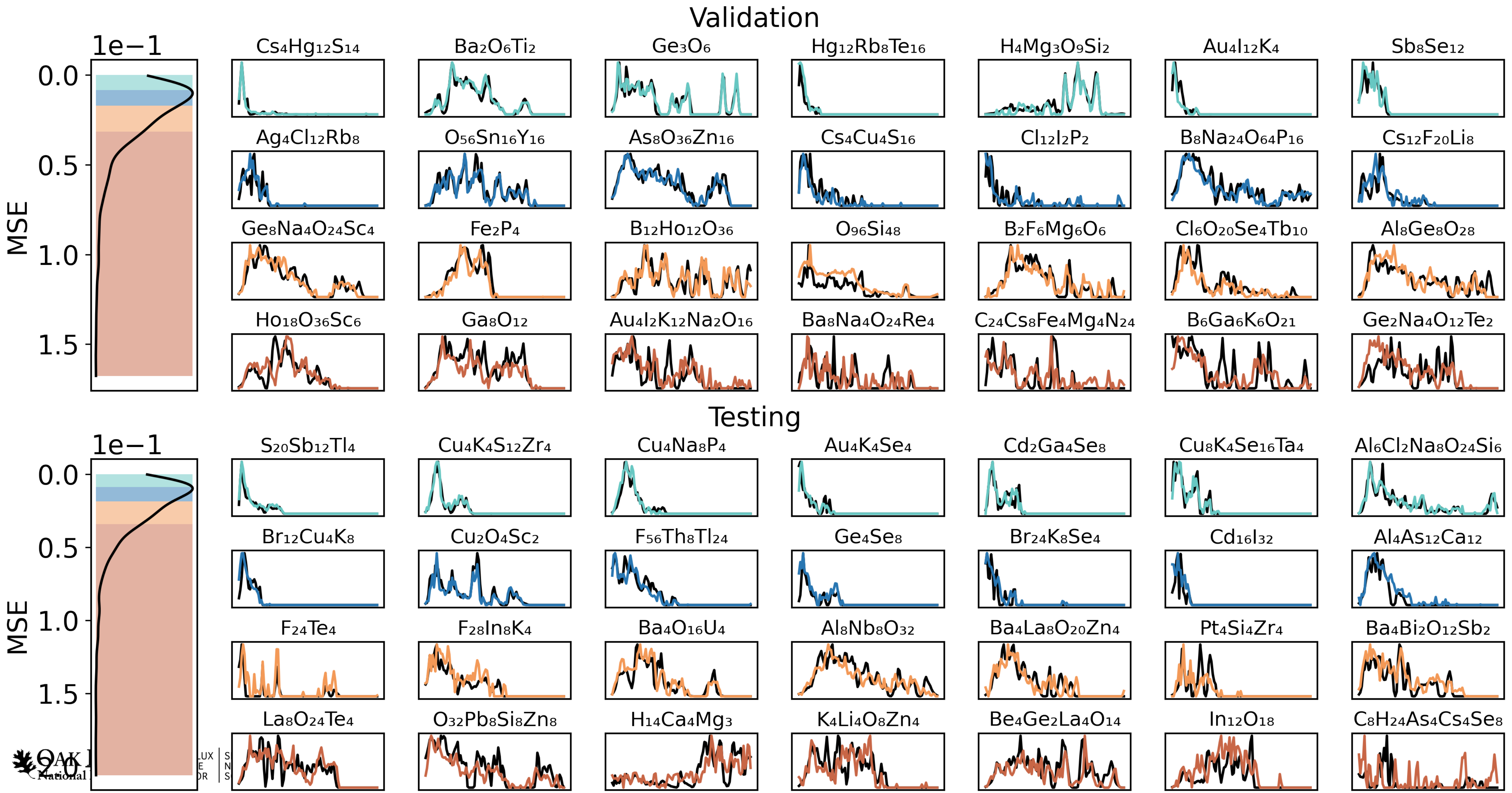
Chen et al. Chem. Phys. Rev. **2**, 031301 (2021)
Chen et al. Adv. Sci. **8**, 2004214 (2021)

From structure to spectra (Inorganic crystals)

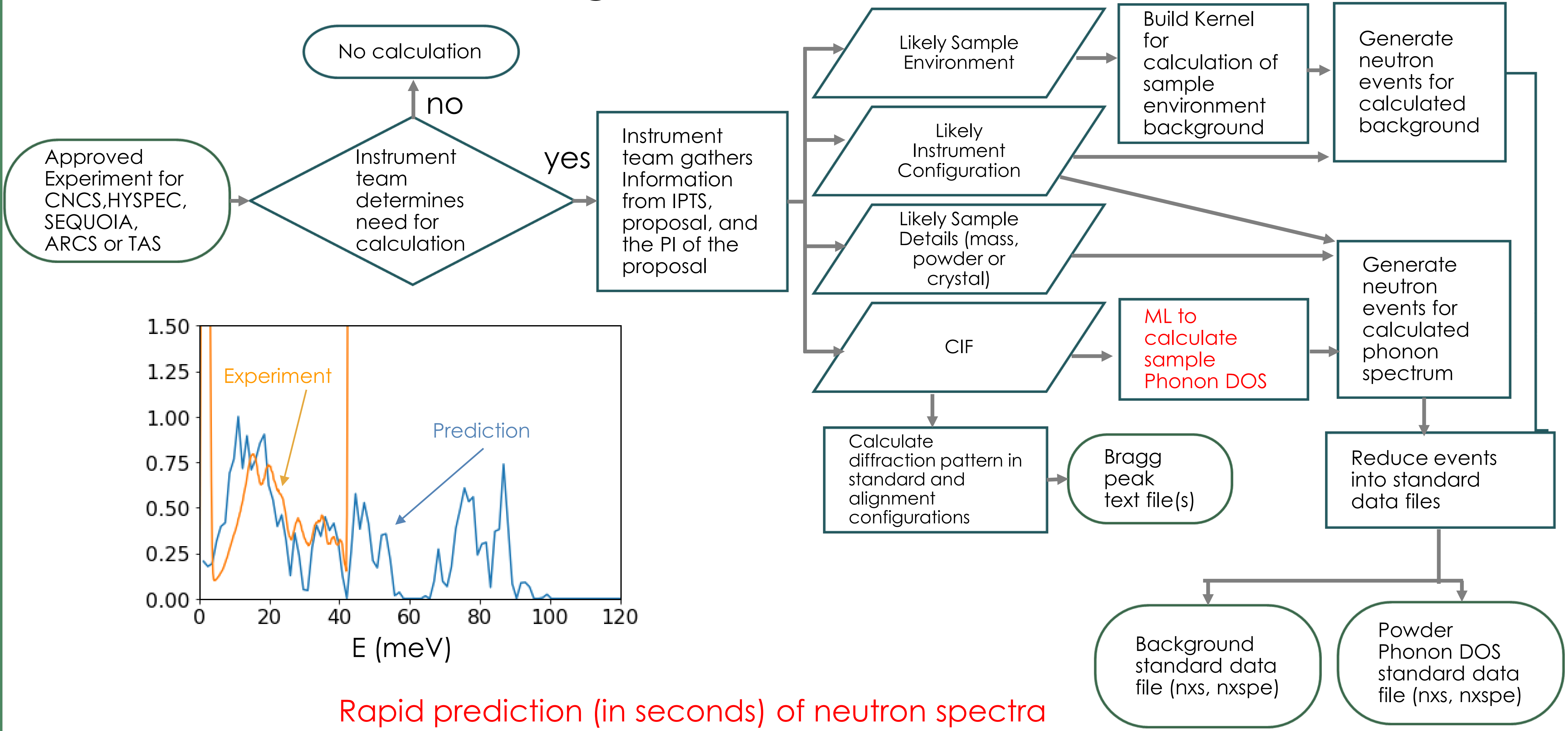
- Materials Project Phonon Database (~10,000 inorganic crystals, 90% training, 5% validation, 5% testing) [http://phonondb.mtl.kyoto-u.ac.jp/]
- Euclidean Neural Network (e3nn) [https://e3nn.org/]
- Simulated INS spectra were generated using VASP/Phonopy and OCLIMAX (10~1000cm^{-1}, 100 data points)



From structure to spectra (Inorganic crystals)



A critical link in the digital twin workflow



Rapid prediction (in seconds) of neutron spectra directly from molecular/crystal structure on a PC, for users with no modeling background.

Credit: Matt Stone

Opportunities

- Access by users either through a web interface or Analysis
- Experiment planning
- Rapid/automated data analysis and interpretation

Thank you!