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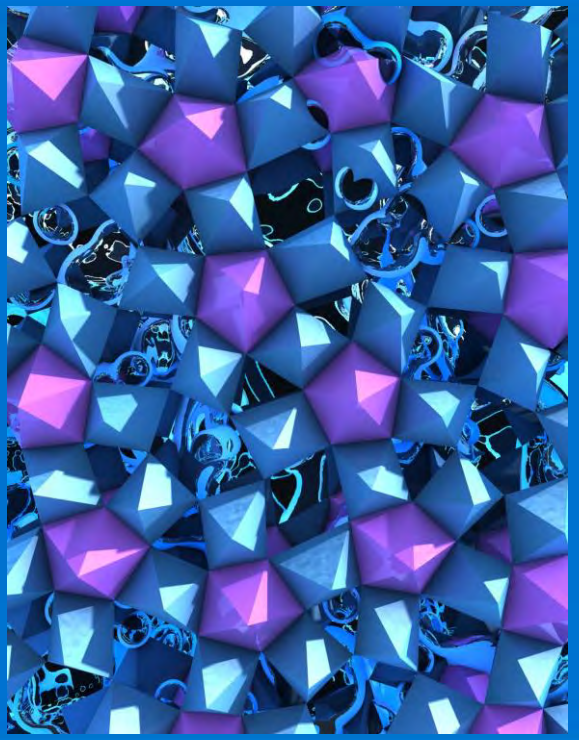
Niobium-based materials for energy conversion and storage



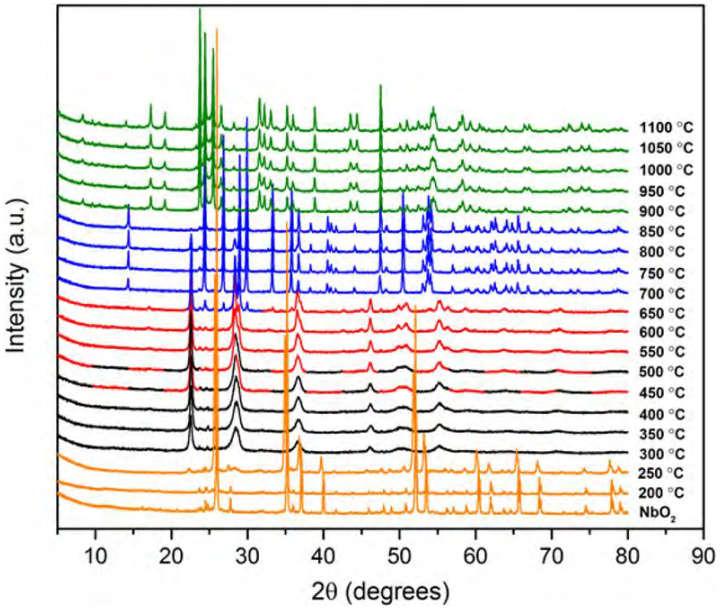
Kent J. Griffith,[1,2] Clare P. Grey,[2] G. Jeffrey Snyder[1]

[1]Northwestern University, Evanston, IL, USA

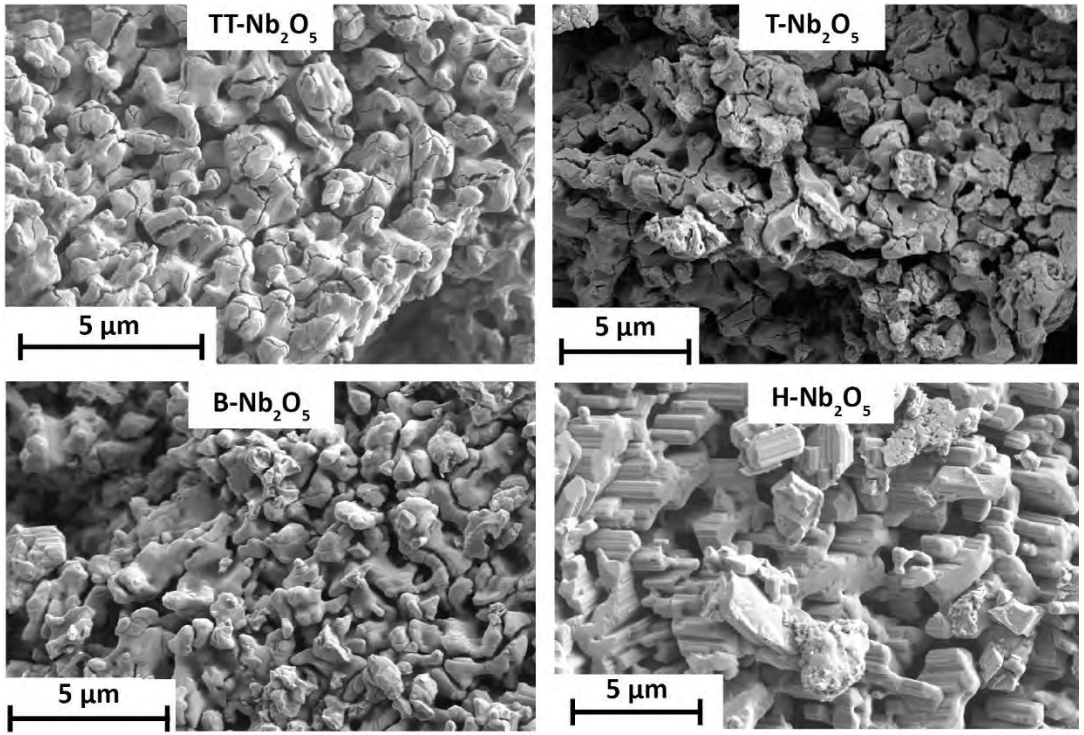
[2]University of Cambridge, Cambridge, UK

24 May 2019

Advanced Structural Characterization of Nb_2O_5

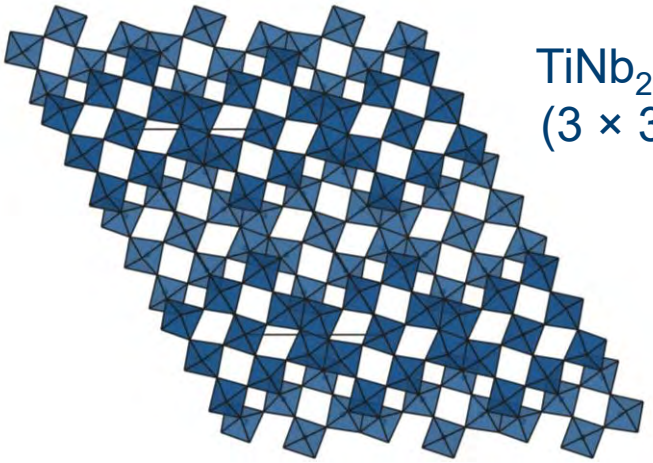


Griffith, K. J. *et al. JACS*, **2016**, *138*, 8888–8899.

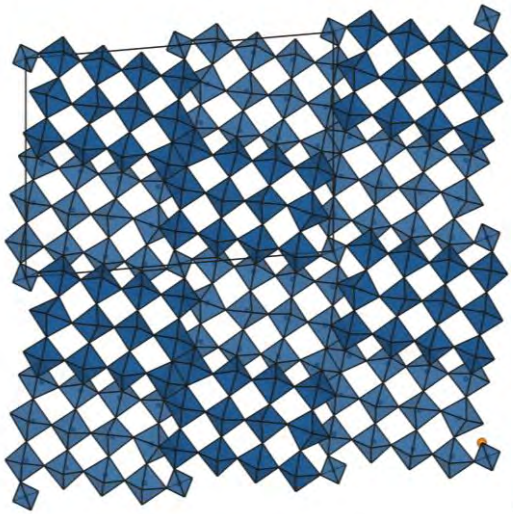


Also, solid-state nuclear magnetic resonance (NMR) spectroscopy,
Particle accelerator studies: neutron diffraction, X-ray spectroscopy, X-ray diffraction

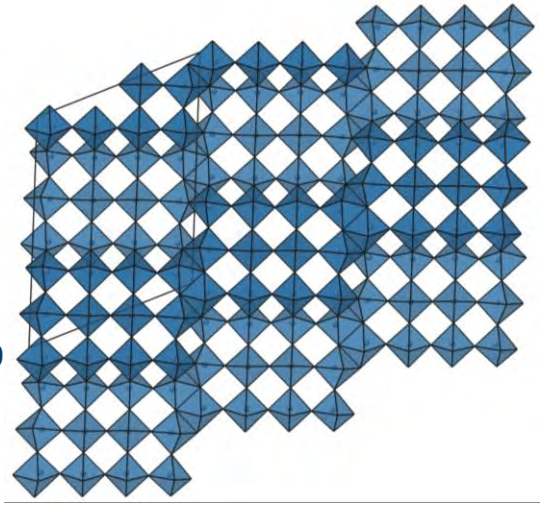
Crystallographic shear (Wadsley–Roth) structure



$TiNb_2O_7$
$(3 \times 3)_\infty$

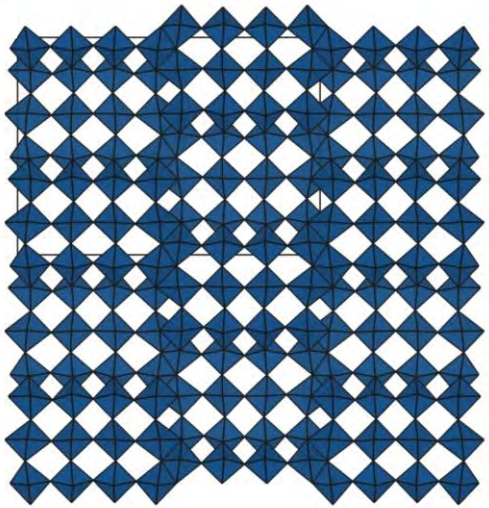


$TiNb_{24}O_{62}$
$(4 \times 3)_2$

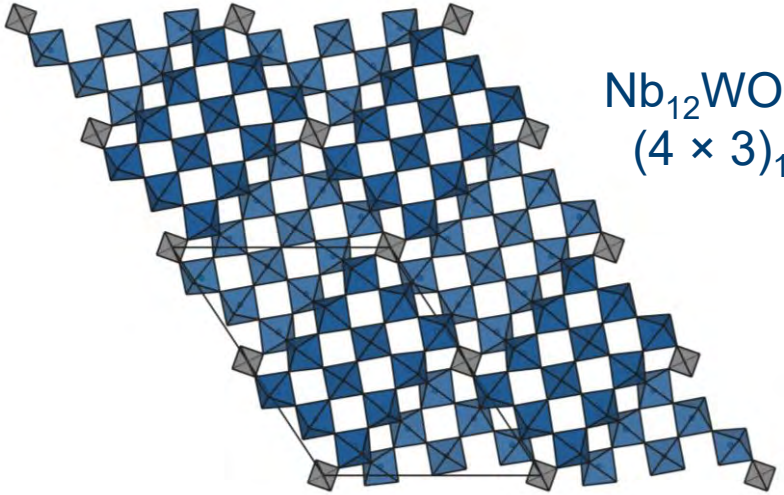


m-$Ti_2Nb_{10}O_{29}$
$(4 \times 3)_\infty$

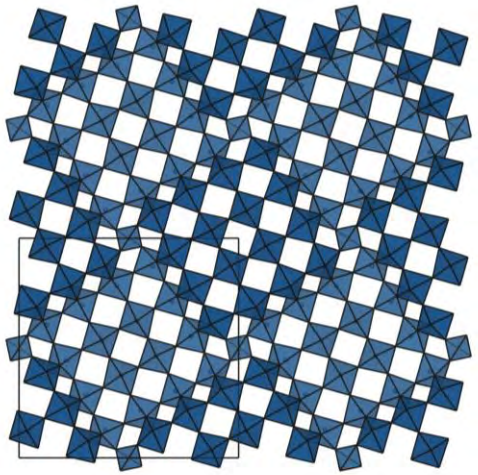
o-$Ti_2Nb_{10}O_{29}$
$(4 \times 3)_\infty$



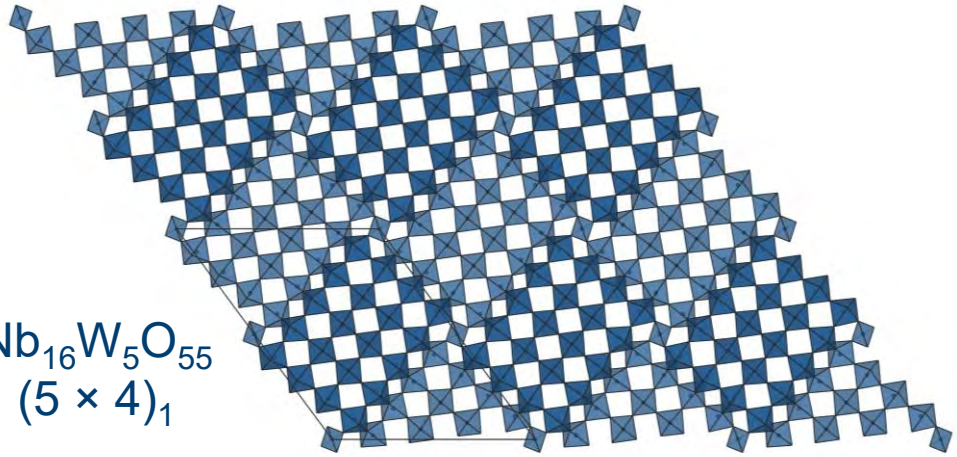
Crystallographic shear (Wadsley–Roth) structure



$Nb_{12}WO_{33}$
$(4 \times 3)_1$

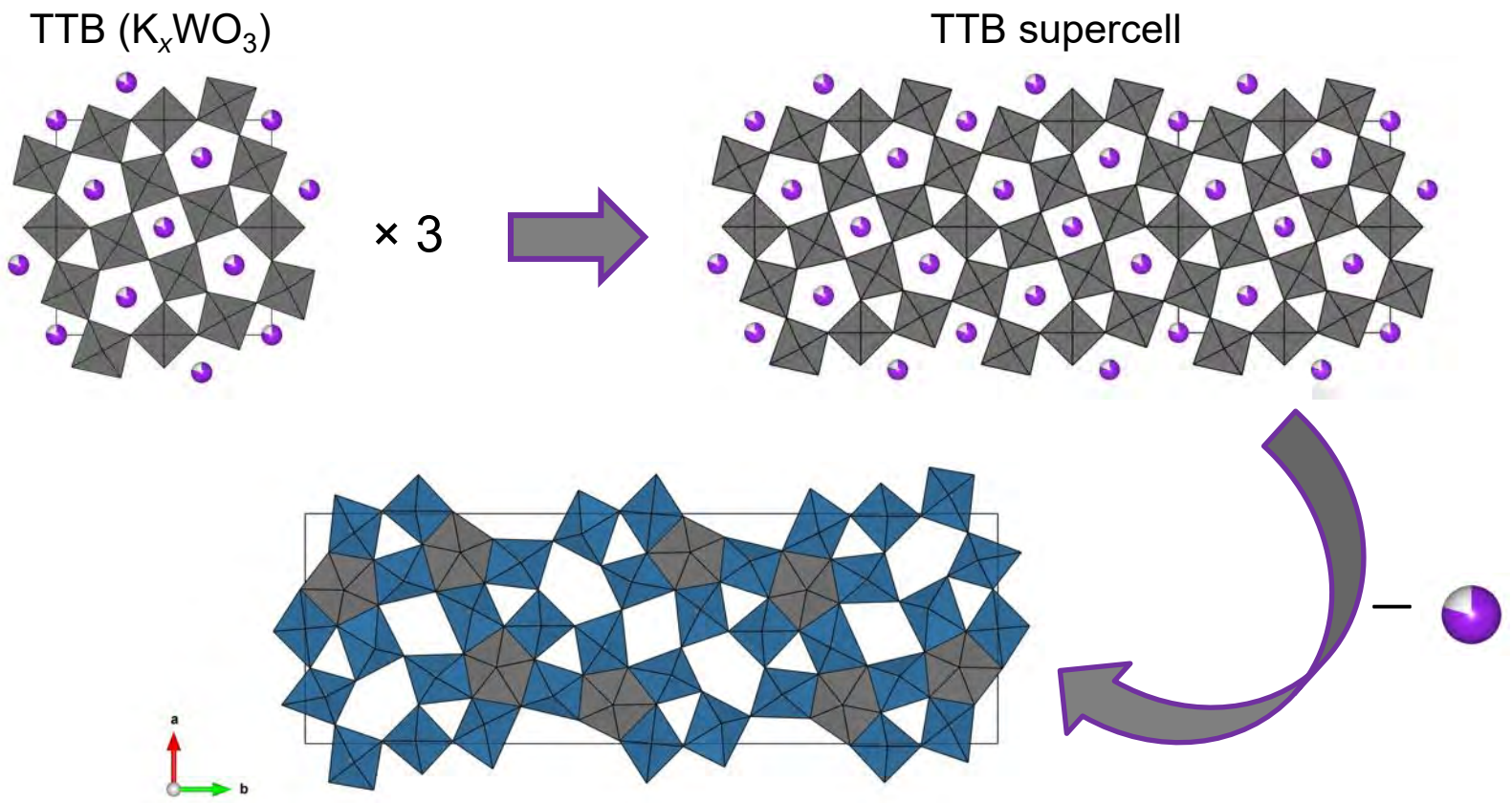


$Nb_{14}W_3O_{44}$
$(4 \times 4)_1$



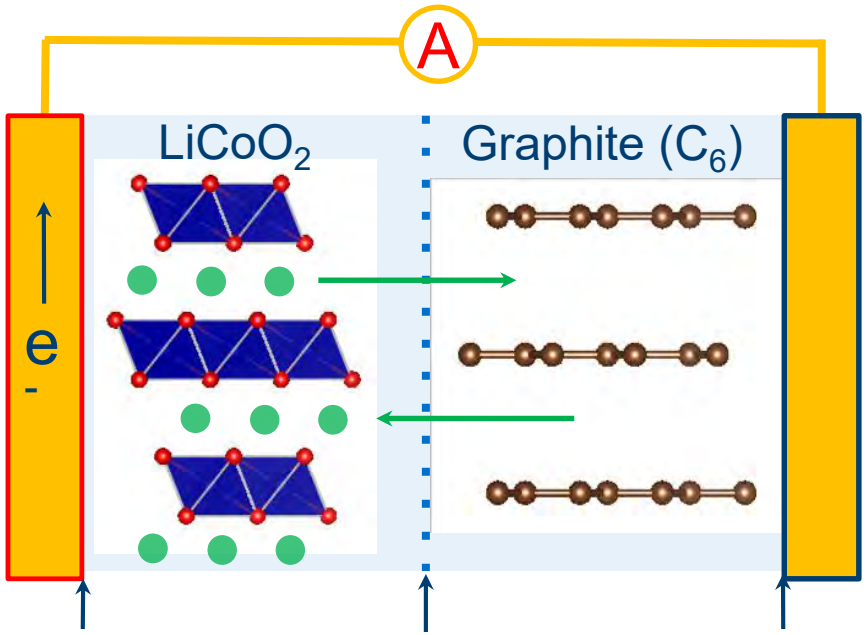
$Nb_{16}W_5O_{55}$
$(5 \times 4)_1$

$Nb_{18}W_{16}O_{93}$ structural analogue of T-Nb_2O_5



$Nb_{18}W_{16}O_{93}$ - distorted TTB superstructure

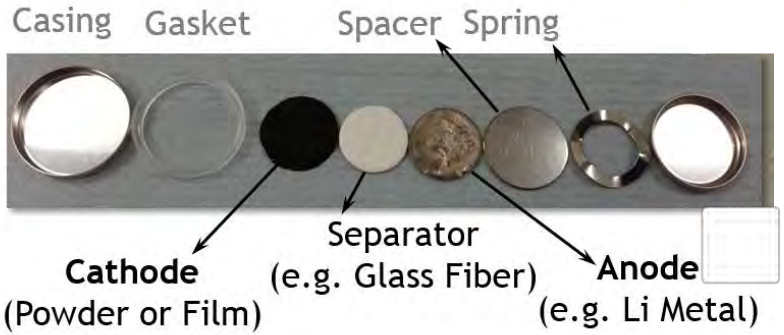
Lithium-ion batteries



Cathode
Positive Electrode

Electrolyte
Liquid or solid

Anode
Negative Electrode



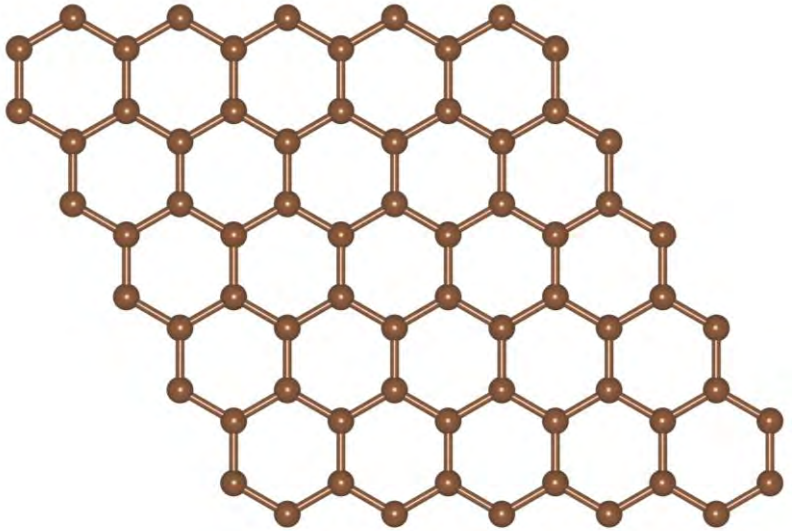
Lithium-ion battery anodes

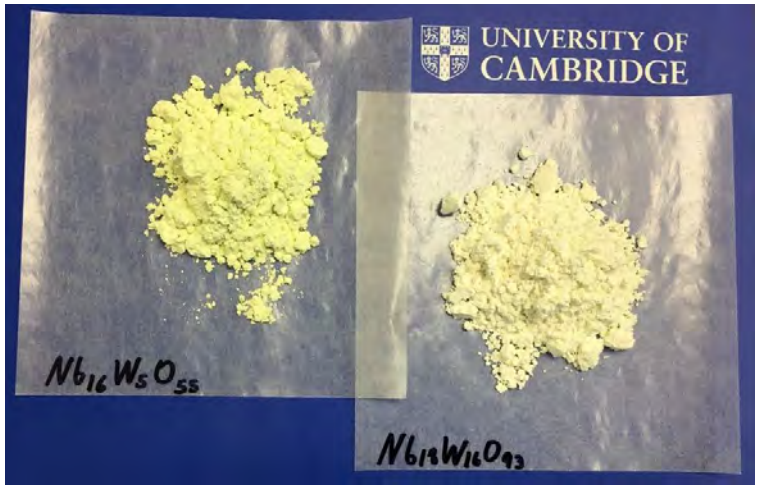
Anodes: 100,000 tons / year

Graphite (97%)

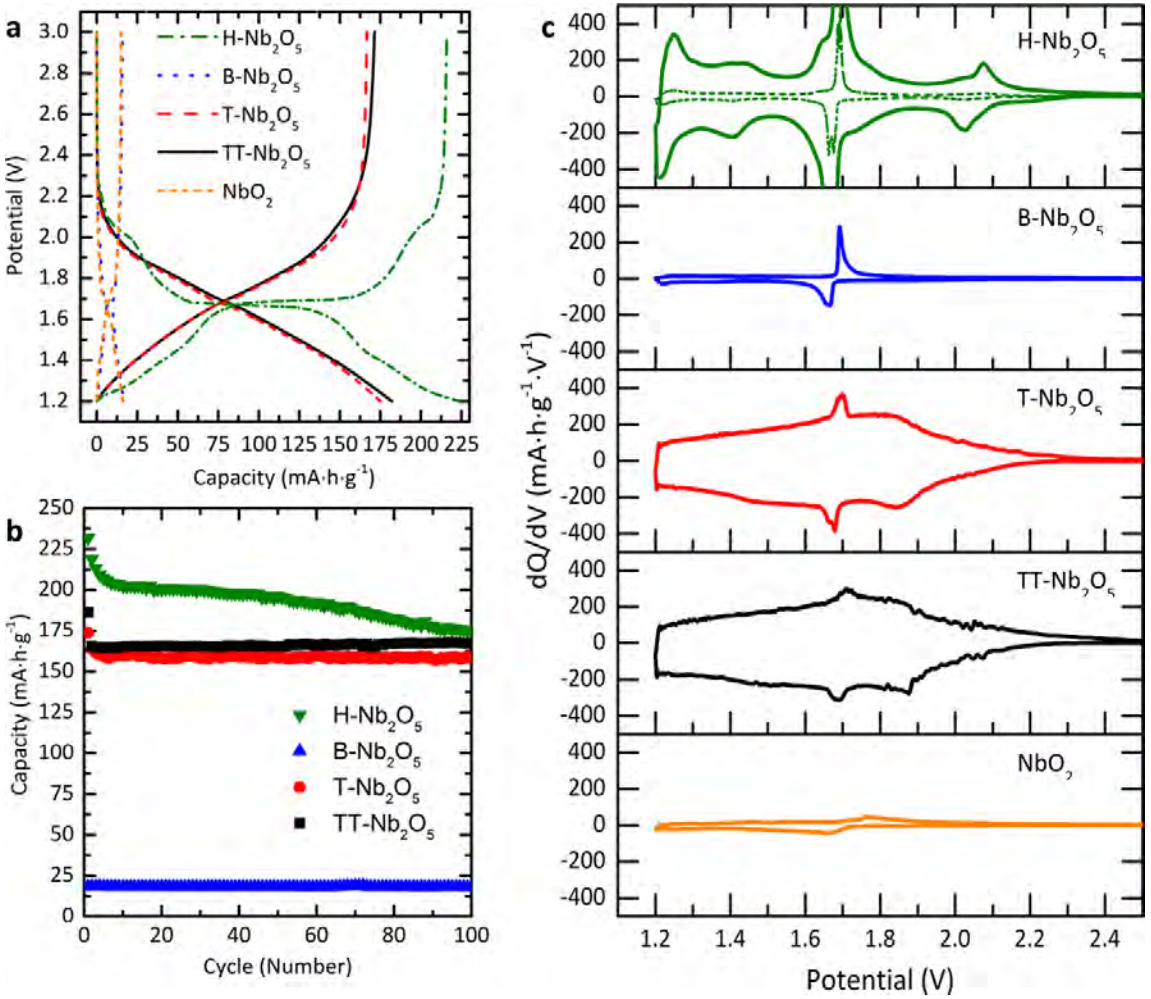
$Li_4Ti_5O_{12}$ (LTO) (3%)

$TiNb_2O_7$ (TNO) / $Nb_{16}W_5O_{55}$ (NWO)



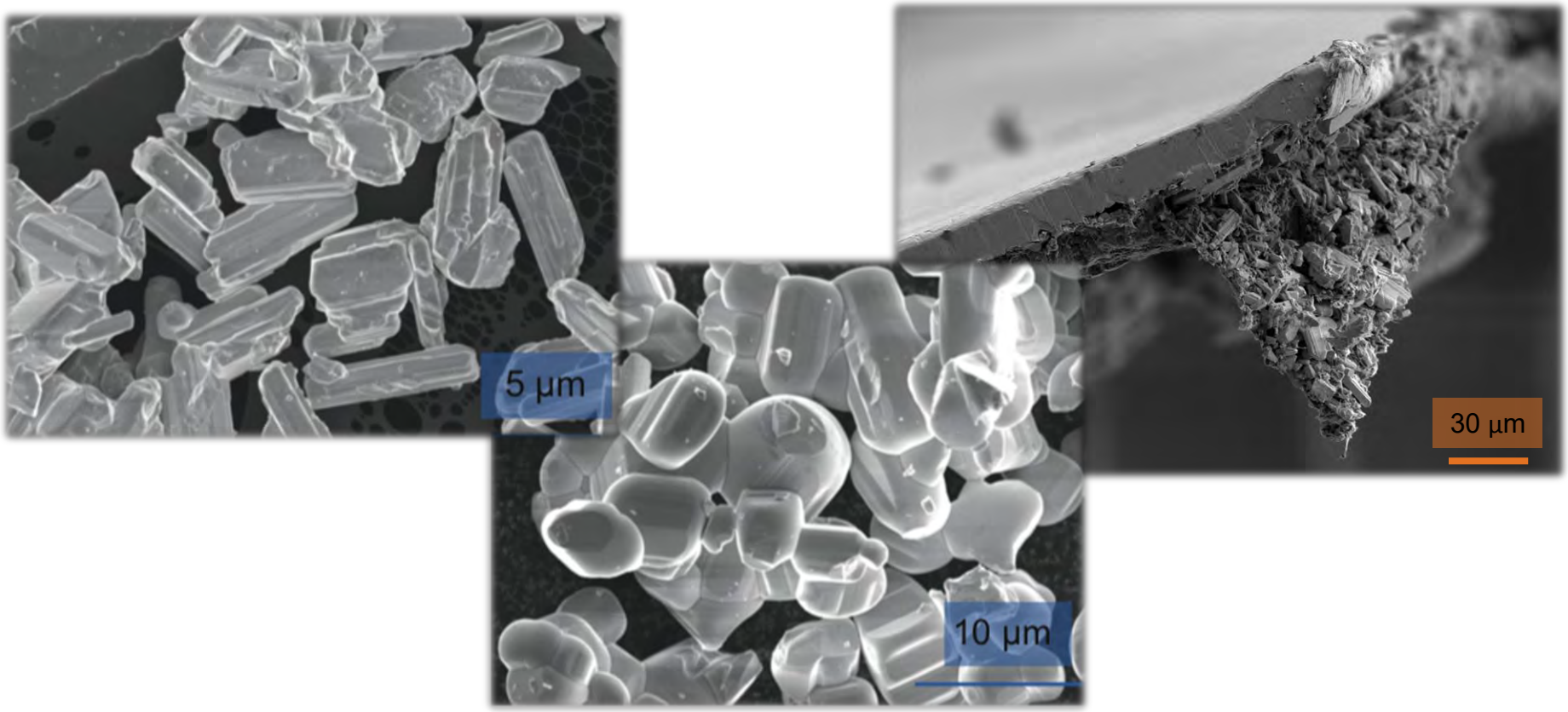


Lithium-ion batteries from Nb_2O_5

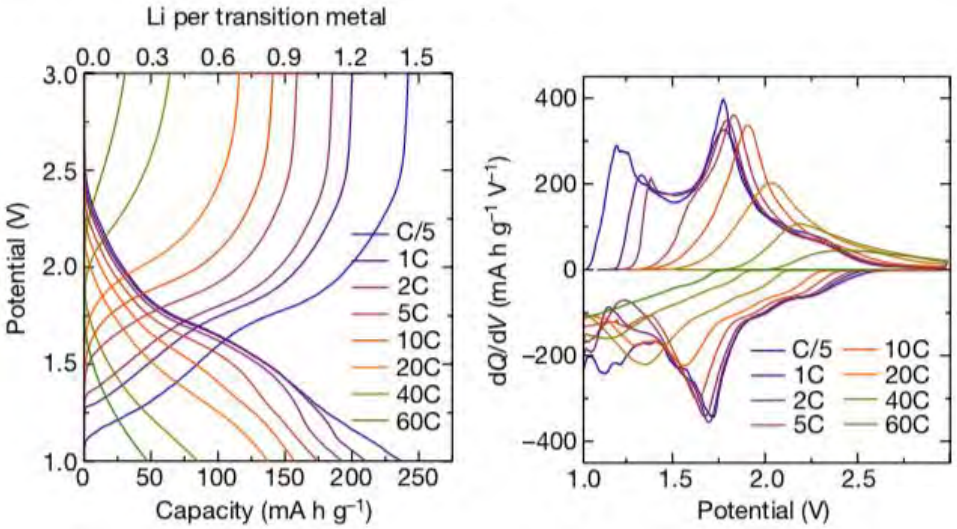


New anode materials: complex mixed metal oxides

Motivation: Bulk high rate performance → fast charging, high power output

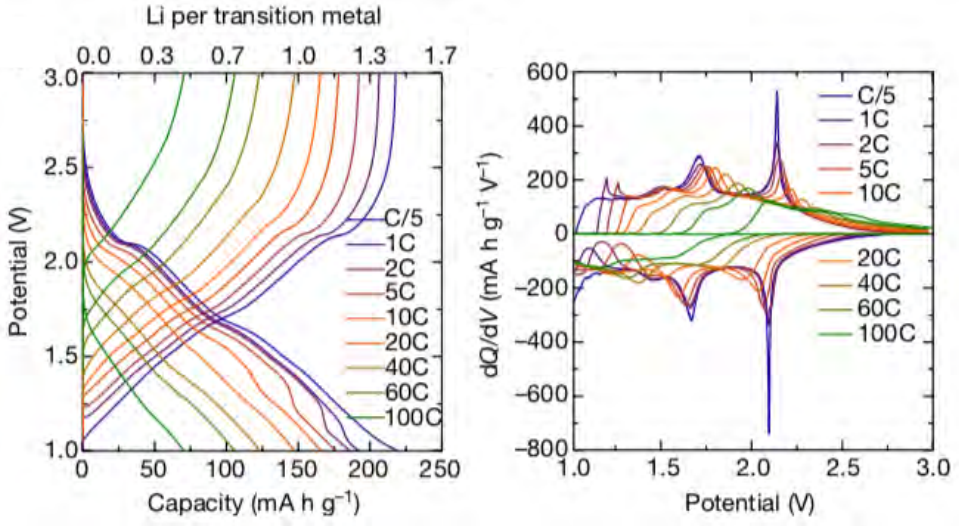


Niobium tungsten oxide electrochemistry



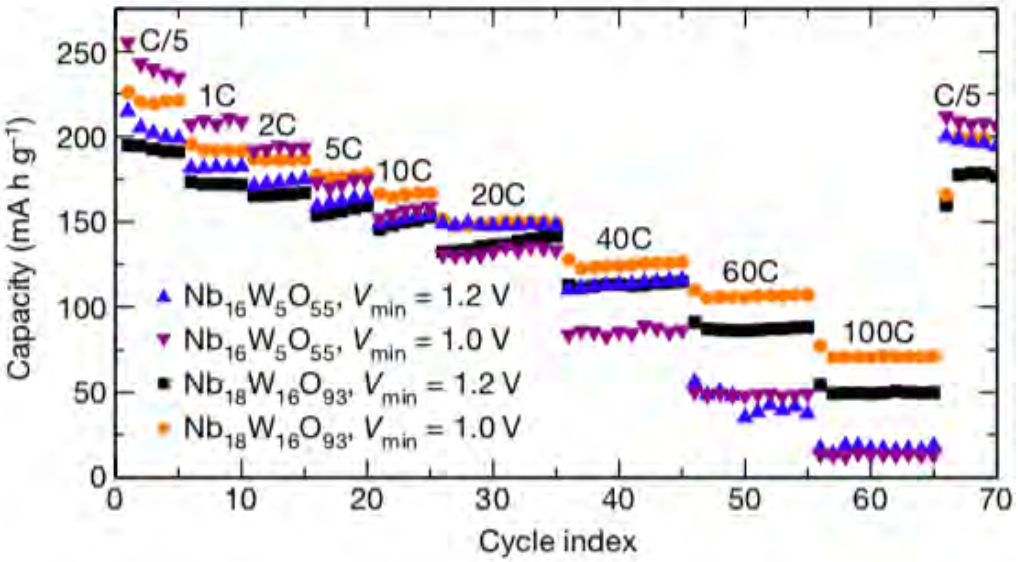
$Nb_{16}W_5O_{55}$

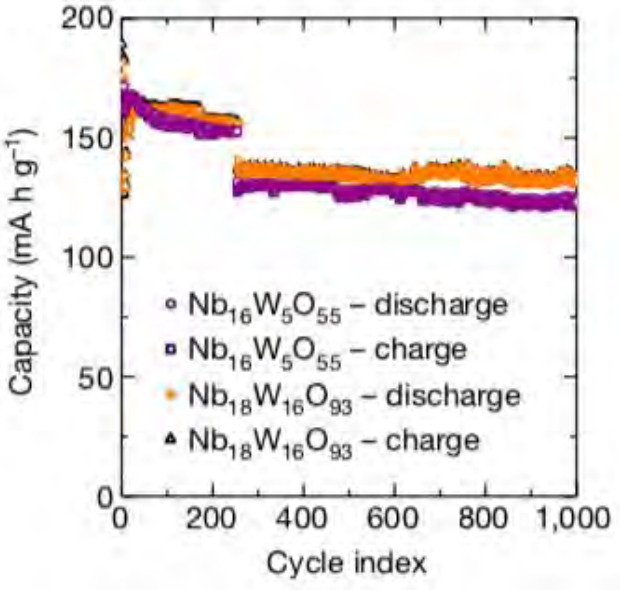
$Nb_{18}W_{16}O_{93}$



Griffith, K. J. *et al. Nature*, **2018**, *559*, 556–563.

Niobium tungsten oxide electrochemistry





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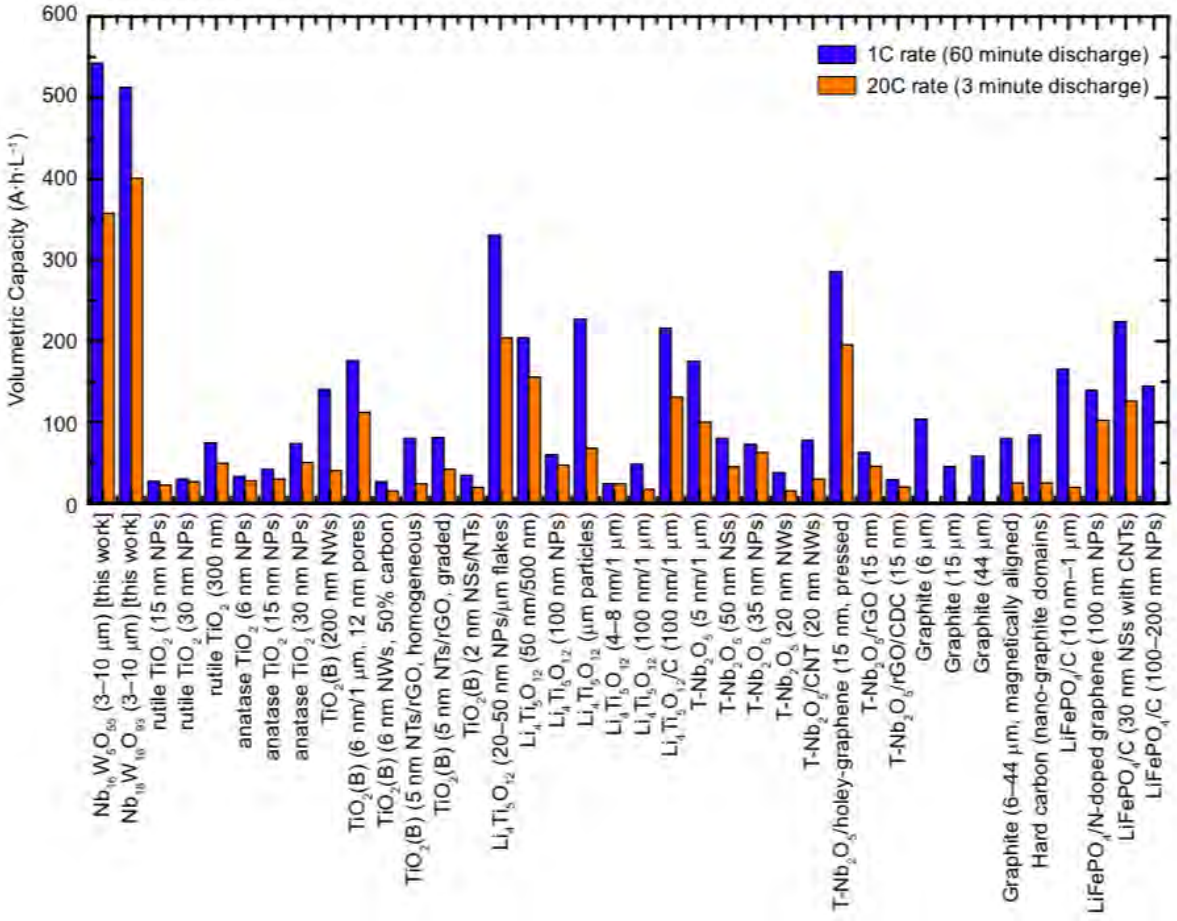
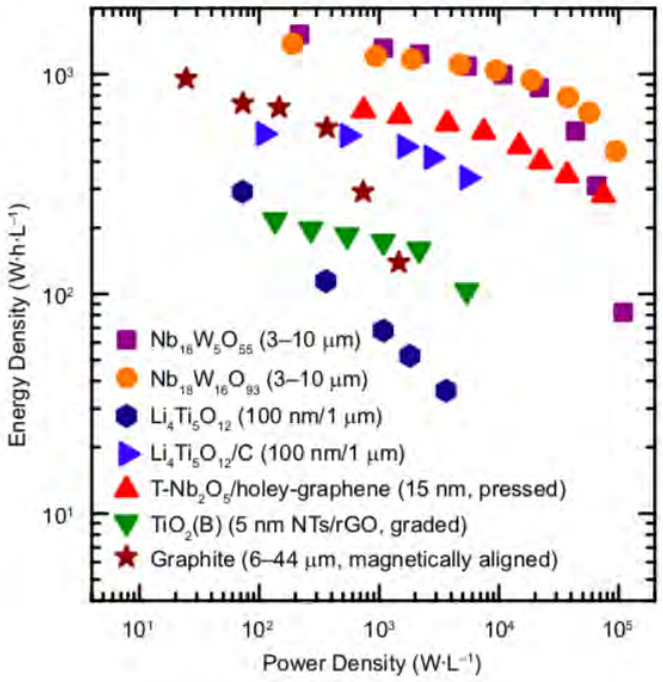
Niobium tungsten oxide electrochemistry

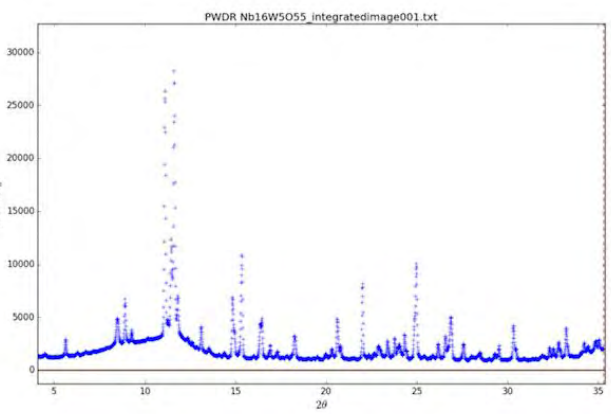


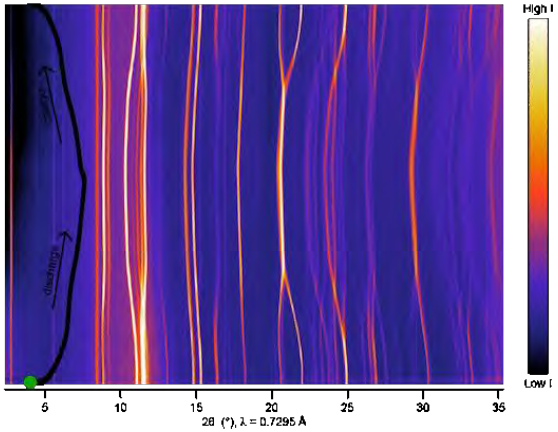
$Q_{volumetric}$ scales with: crystal density, microstructural density, proxy: Li/TM (Li/atom)



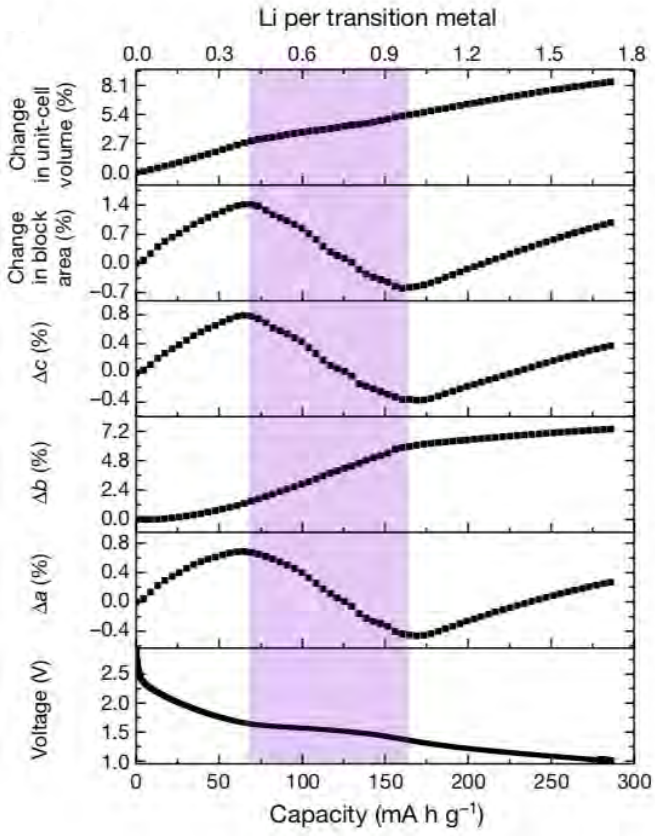
Operando high-rate structure evolution

$Nb_{16}W_5O_{55}$



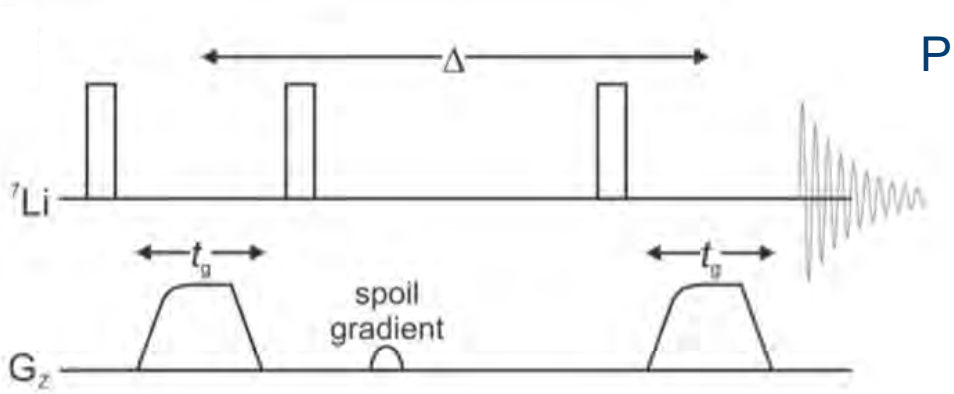


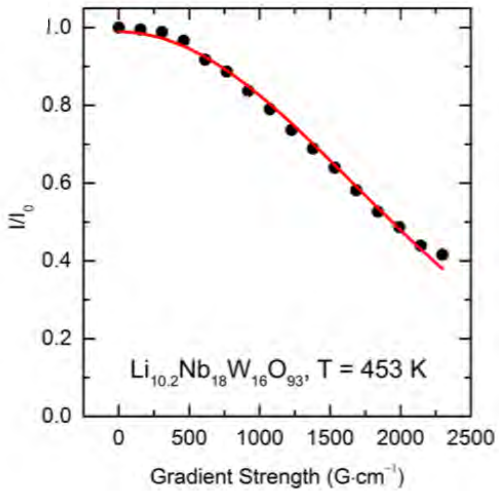
high-rate *operando* diffraction

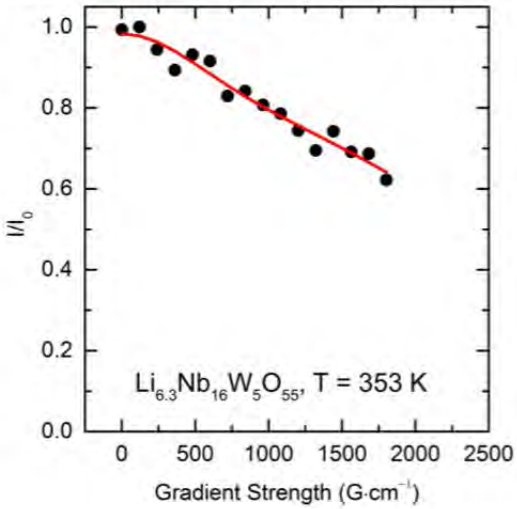


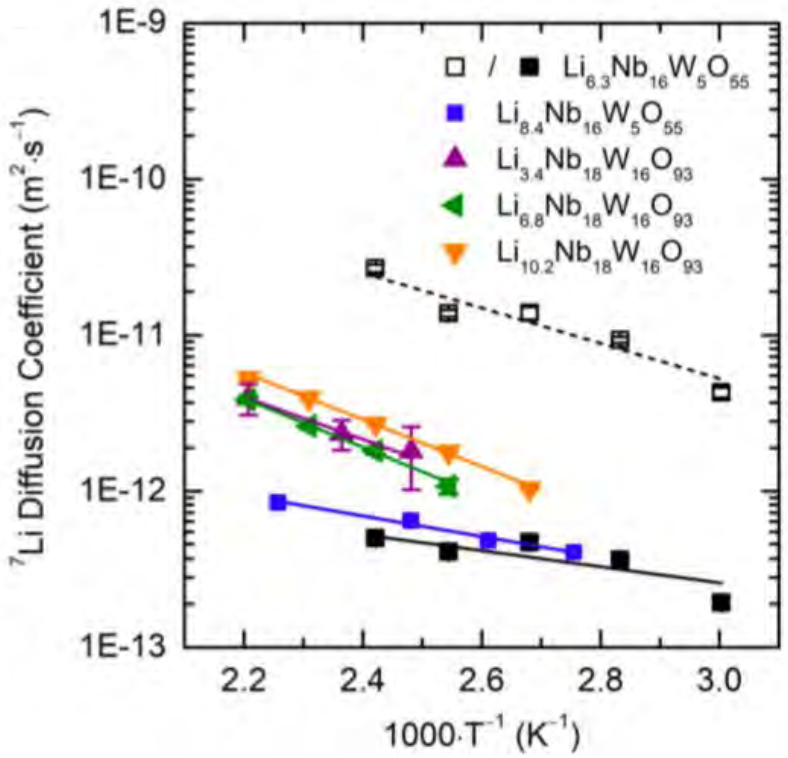
Pulsed field gradient NMR Spectroscopy

PFG NMR: Direct, real-space Li^+ diffusion in a mixed ionic–electronic conductor



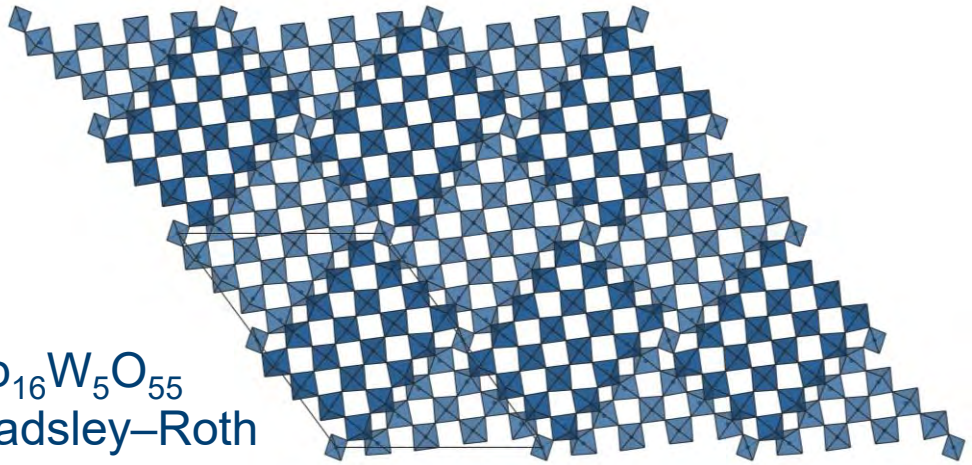






Griffith, K. J.; Wiaderek, K. M.; Cibin, G.; Marbella, L. E.; Grey C. P. *Nature*, **2018**, *559*, 556–563.

Complex mixed metal oxides

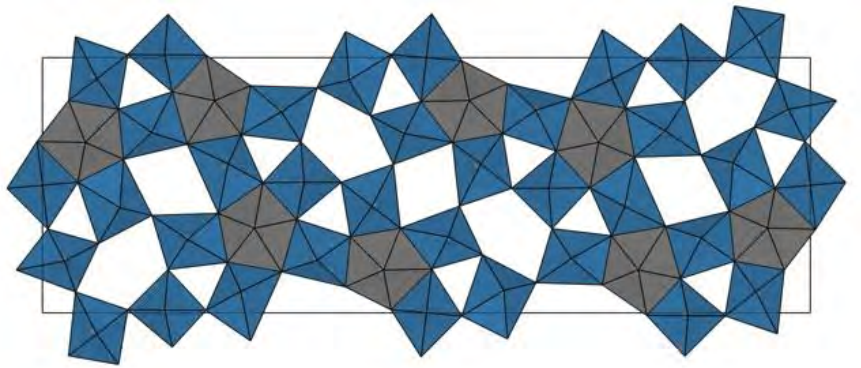


$Nb_{16}W_5O_{55}$
Wadsley–Roth

shear planes

frustrated polyhedral networks

locked tunnels



$Nb_{18}W_{16}O_{93}$ - distorted TTB superstructure

Open diffusion pathways for rapid ionic transport

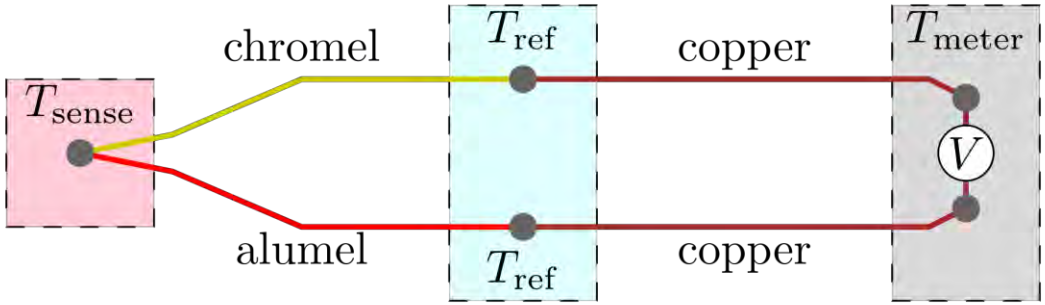
Multiredox capability from both metal cations (& prevents ordering)

Thermoelectric energy conversion

Seebeck effect (thermoelectric effect): a temperature difference (ΔT) generates a voltage (ΔV) across a wire

Thermocouple: uses thermoelectric effect to measure temperature

- ovens/kilns/furnaces
- pilot light on gas heaters
- home & office thermostats
- wide industrial applications

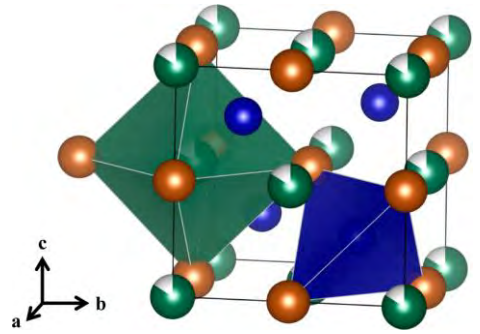


Thermopile: combine thermoelectric devices in series to generate usable voltage to power electronics

Thermoelectric energy conversion

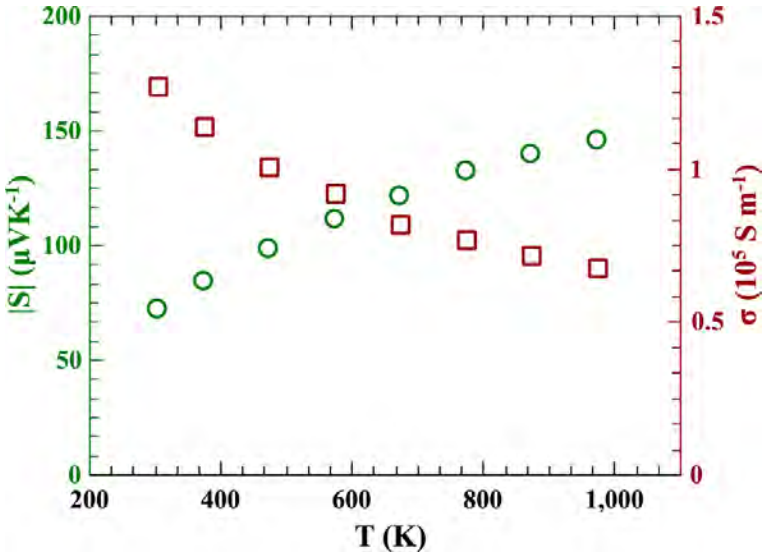
K-type thermocouple (most common)

- Chromel and alumel alloys (>90% nickel)
- Sensitivity/power 41 $\mu V \cdot K^{-1}$ (Seebeck coefficient)



Niobium-based semiconductor alloy

- Niobium + metal + antimony
- Sensitivity/power > 150 $\mu V \cdot K^{-1}$
  - Three times higher power



Snyder et al. *Chemistry of Materials*, **2017**, *29*, 1210–1217.

Acknowledgements

Professor Clare Grey (Cambridge)

Professor Jeff Snyder (Northwestern)

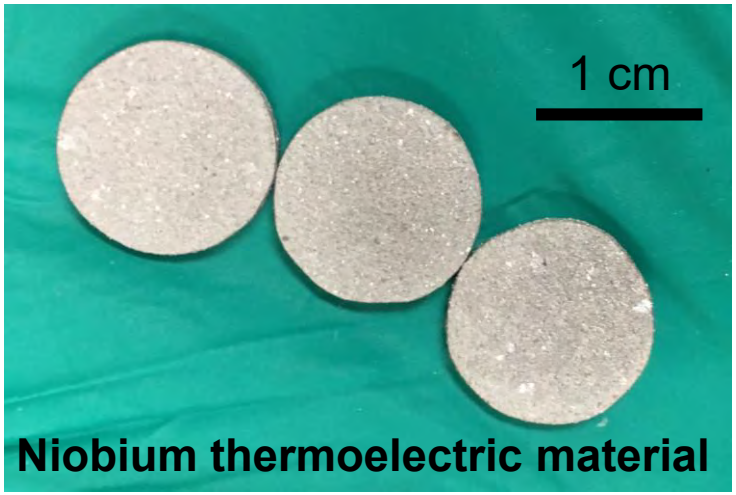
Dr. John Griffin (Lancaster University)

Dr. Alex Forse (UC Berkeley)

Professor Lauren Marbella (Columbia University)

CHURCHILL SCHOLARSHIP
SCIENCE/MATHEMATICS/ENGINEERING

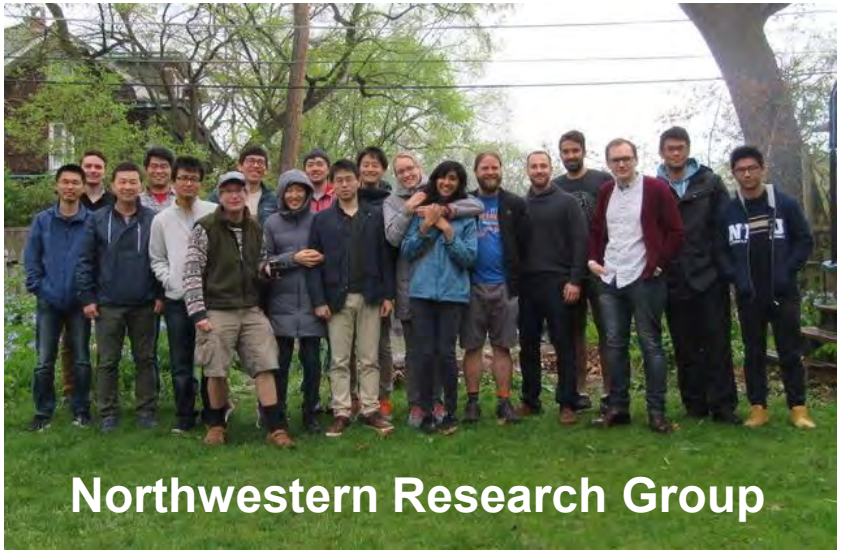
Herchel Smith Scholarship



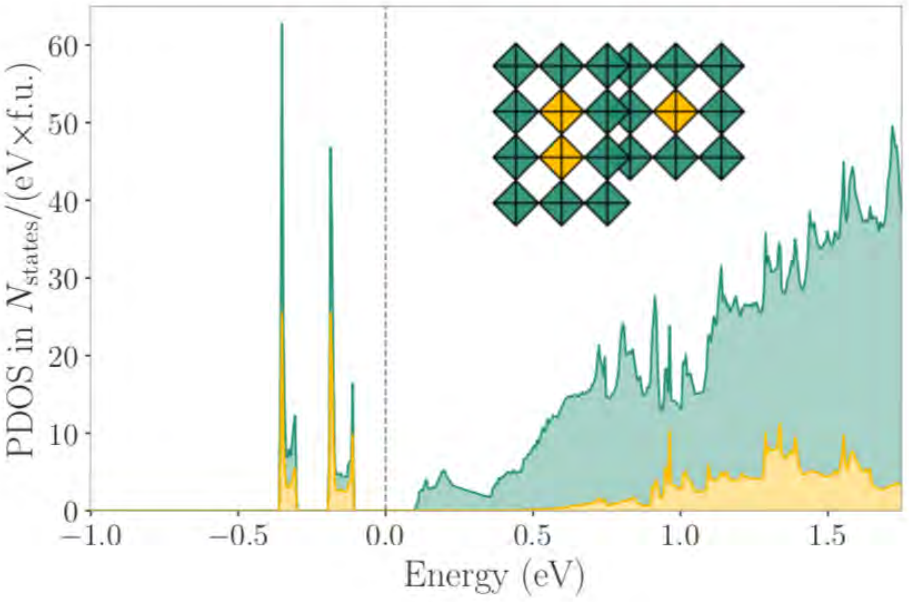
Niobium thermoelectric material

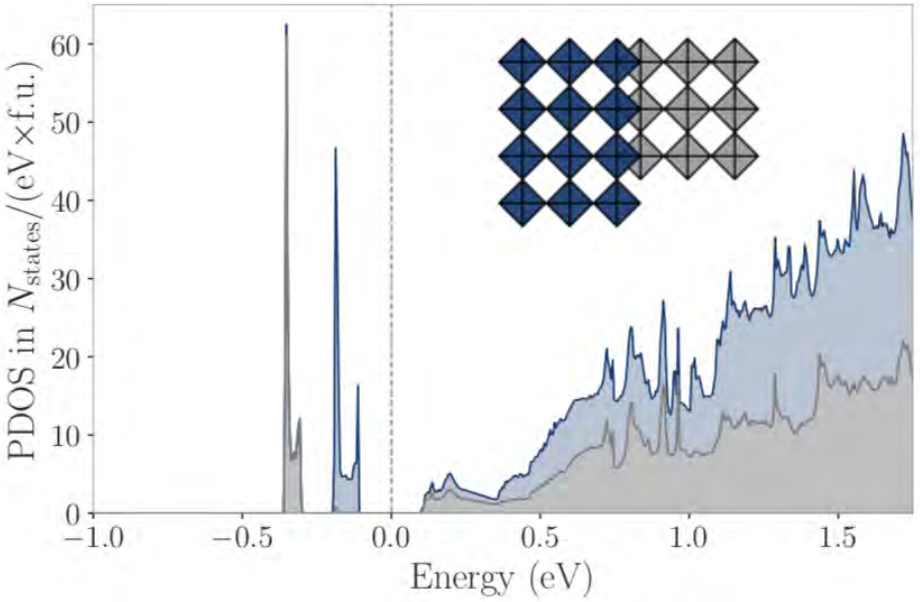
STFCBatteries.org

Acknowledgements



Electronic behavior





Kocer, Griffith *et al. Physical Review B*, **2019**.