The Local Spectroscopy Data Infrastructure

The Materials Project

NSF CSSI PI Meeting, Seattle, WA, Feb. 13-14, 2020

NSF Award # 1640899

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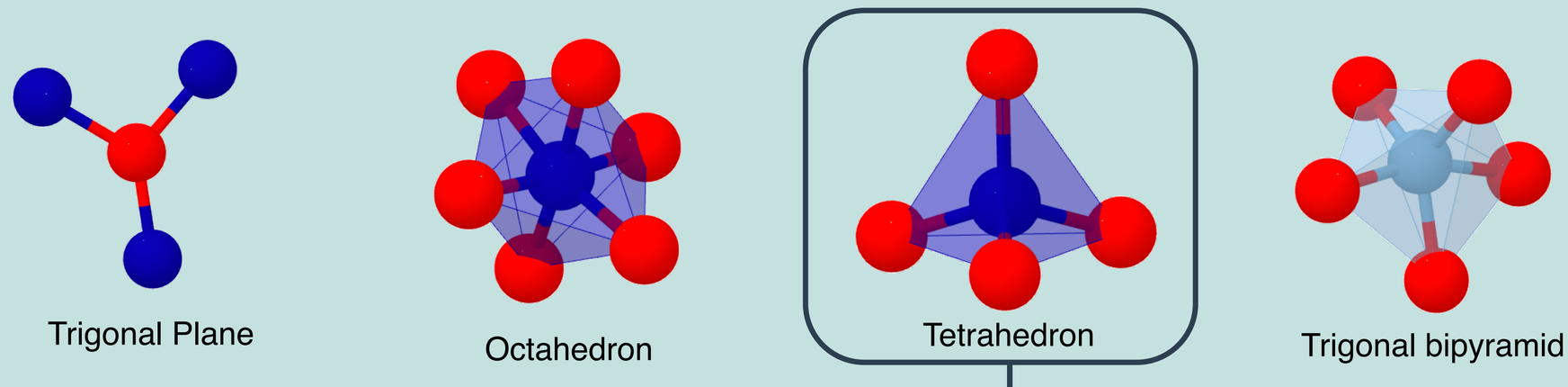
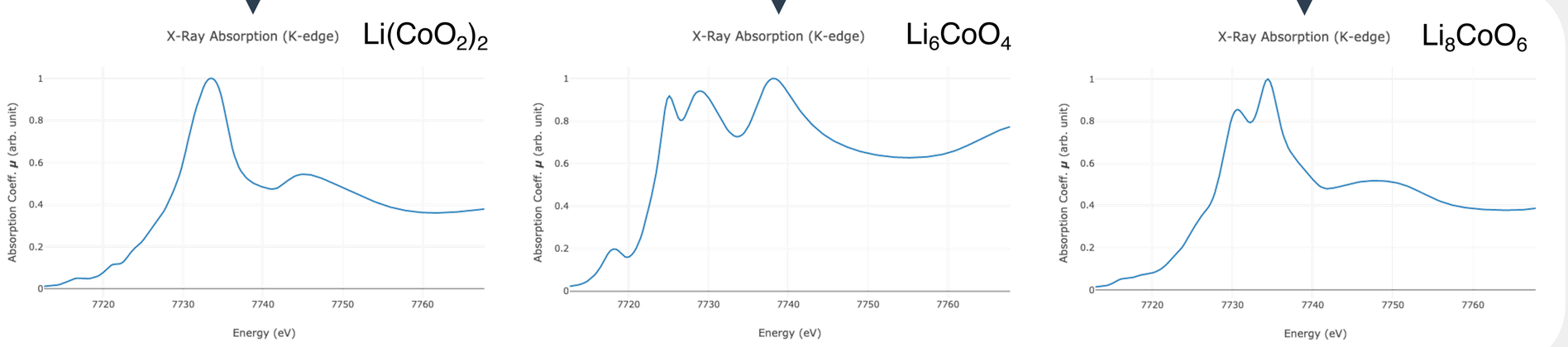
Local atomic environments are often described by the bonding topology of the first nearest neighbor atoms in a material. These motifs provide a geometric construct for material scientists to rationalize, design and tweak the performance of energy materials such as battery cathodes and solar photovoltaic absorbers

The variation and distribution of local atomic environments controls the functionality of inorganic materials



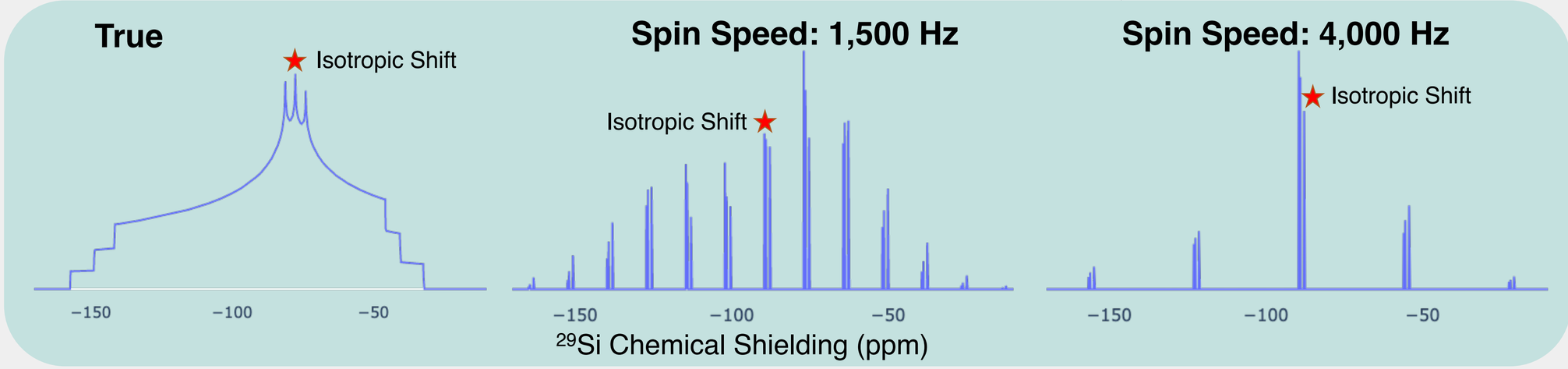
Methods such as X-ray Absorption Spectroscopy (XAS) can differentiate minute variations in local atomic environments **even in all tetrahedral coordination**



Even though cobalt is coordinated with 4 oxygen atoms to form a tetrahedron in all three lithium-containing materials to the left, the minute distortions in tetrahedral coordination can be directly interrogated by changes in their XAS spectra as demonstrated by these computed spectra

Often these spectroscopy techniques, such as **solid state Nuclear Magnetic Resonance (ssNMR),** are labor- and time-intensive with **significant optimization of experimental parameters to achieve useful results**

The spectra to the right demonstrate the effect of the spin-speed in ssNMR for 4-coordinated silicon, which can significantly reduce measurement durations, but might not yield sufficient information to identify the local atomic environment. A spin speed of 4,000 Hz is sufficient to identify the isotropic shift but not the full manifold of the spectrum.



Despite the importance of these techniques and the nearly infinite variation in local atomic environment, known reference spectra for XAS and ssNMR exist primarily in printed anthologies

The Local Spectroscopy Data Initiative is building a Computational Database of XAS and ssNMR spectra to accelerate designing next generation materials

High Throughput Computational Simulation Stack

119,856	145,594	39,544	9,397
K-Edge XANES Spectra (1M CPU Hours)	K-Edge EXAFS Spectra (50K CPU Hours)	L-Edge XANES Spectra (200K CPU Hours)	^{29}Si Chemical Shielding Tensors (16M CPU Hours)

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