The XANES Inverse Project

W**ho?**
Matt Carbone, Reichman Group

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Wednesday, February 27\textsuperscript{th}, 2019 at 5:15 pm

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7\textsuperscript{th} Floor Lounge, 711 Havemeyer

A**bstract**
X-ray absorption near-edge structure (XANES) spectroscopy is a robust and element-specific tool for probing the atomic structure of materials. Traditional spectroscopy methods work in the forward direction by simulating XANES spectra from atomic models. Here, we present the opposite: a computational method that predicts information about the local structural geometry from XANES spectra, in which the so-called inverse problem is solved using supervised machine learning. The robustness and fidelity of the method are demonstrated by an average F1 classification accuracy of 86% on a database consisting of the K-edge XANES spectra of hundreds of materials across eight 3d transition metal families.

Plenty of pizza will be provided.