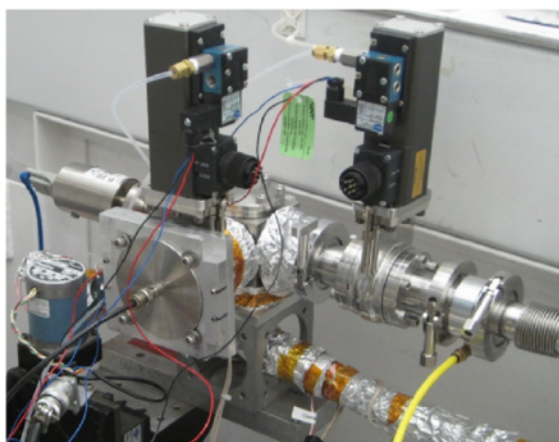


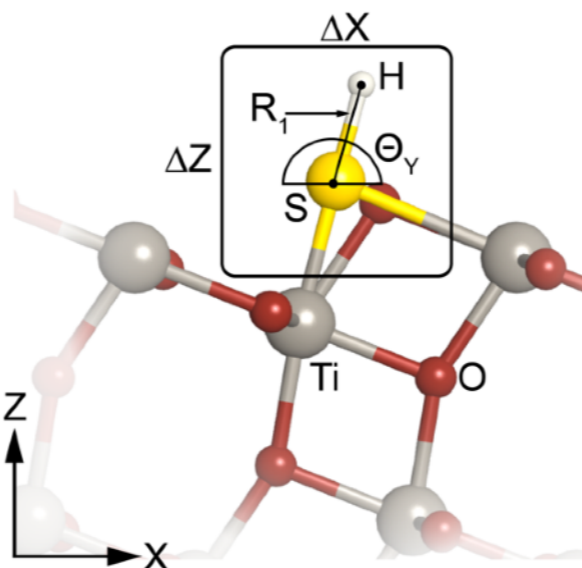
In situ XANES



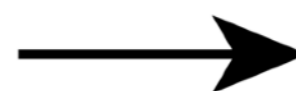
Prepare simulations



Ab initio simulations

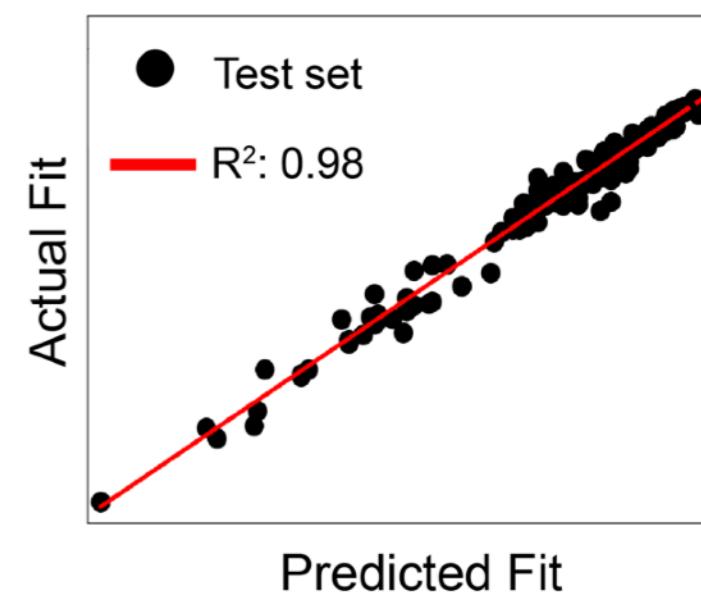
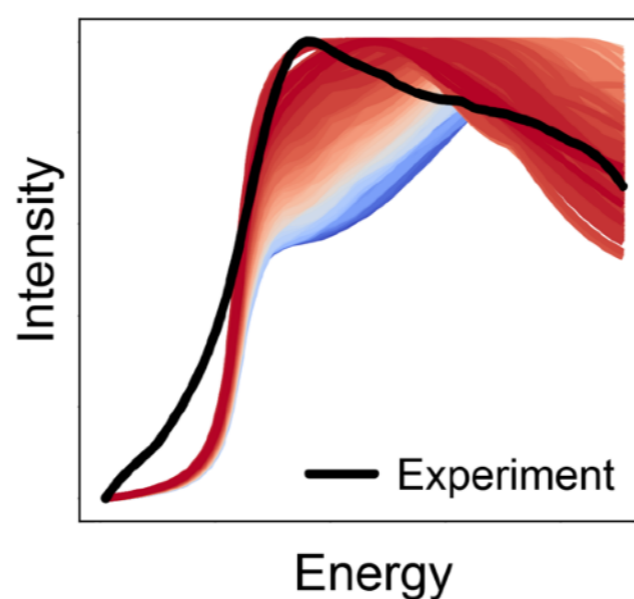
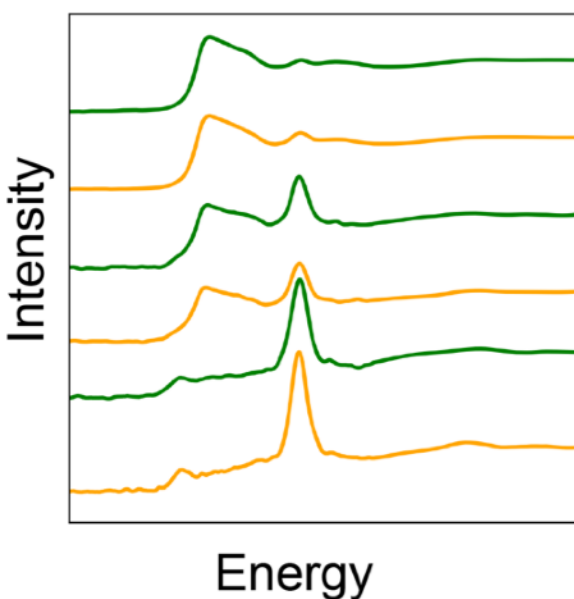


Analyze data



Machine learning

Parameters						Target
ΔX_s	ΔY_s	ΔZ_s	$\Delta \Theta_x$	$\Delta \Theta_y$	ΔR_1	Fit
Training, validation and test sets						



Reference: Trejo, O.; Dadlani, A. L.; De La Paz, F.; Acharya, S.; Kravec, R.; Nordlund, D.; Sarangi, R.; Prinz, F. B.; Torgersen, J.; Dasgupta, N. P. Elucidating the Evolving Atomic Structure in Atomic Layer Deposition Reactions with in Situ XANES and Machine Learning. *Chem. Mater.* **2019**, 31 (21), 8937–8947.