ELUCIDATING, ANALYZING, AND DESIGNING SPECTROSCOPIES: LEVERAGING THEORY AND CHEMICAL INTUITION TO GET THE MOST OUT OF MACHINE LEARNING

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Advances in machine learning are pushing the forefront of what can be simulated and understood about the nature of chemical systems, offering intriguing possibilities for developing new chemical insights in spectroscopies ranging from NMR, to multidimensional electronic spectroscopies, and the recently introduced impulsive nuclear x-ray scattering. In this talk I will present our latest developments showing how machine learning's potential to simulate, analyze and design spectroscopic experiments can be maximized by building chemical intuition and theoretical insights into the underlying frameworks.