

CAPTURING, PREDICTING, AND UNDERSTANDING OPTICAL SIGNALS: HARNESSING MACHINE LEARNING TO TACKLE ENERGY DISSIPATION IN THE CONDENSED PHASE

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While optical spectroscopies provide an essential and ever-expanding toolbox for probing and elucidating how materials absorb, transport, and dissipate energy, accurately predicting their signals remains a formidable challenge to theory. By drastically expanding our ability accurately and efficiently simulate complex systems and their dynamics, machine learning techniques are opening fascinating possibilities for the simulation and analysis of various spectroscopies. In this talk, I will focus on our latest advances showing how one can exploit chemical intuition to combine machine learning techniques with robust theoretical frameworks to faithfully capture and interpret energy transport pathways encoded in optical signals.