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**Dynamics and Structure of Disordered Peptides from Two-Dimensional Infrared Spectroscopy** MIKE REPPERT, JOSHUA LESSING, CHUNTE PENG, KEVIN JONES, CARLOS BAIZ, ANDREI TOKMAKOFF, Department of Chemistry, Massachusetts Institute of Technology — Two-dimensional infrared (IR) spectroscopy is a powerful tool for investigating the ultra-fast dynamics and association of complex biological macromolecules such as proteins and DNA. In addition to the improved spectral discrimination afforded by a two-dimensional spectrum, the ultra-fast time-resolution inherent to the technique provides unique insight (unobtainable by standard linear IR measurements) into the time-scales of macromolecular conformational fluctuations, particularly for intrinsically disordered systems. Here we discuss the use of accurate line shape modeling of peptide amide I vibrations as an advanced method for extracting structural and dynamic information from experimental spectra. The mixed quantum-classical model makes use of standard MD trajectories and a parametrized site energy and coupling map as inputs for excitonic calculations of the delocalized amide I vibrations. We present examples of the application of this method to extract site-specific structural information (such as hydrogen bond number and turn conformation) as well as insight into conformation dynamics and time-scales from experimental data for disordered peptides.

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