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**Achiral and Chiral Sum Frequency Generation Spectroscopy of Peptides** JOSHUA CARR, LU WANG<sup>1</sup>, JAMES SKINNER, University of Wisconsin at Madison — In vibrational sum-frequency generation (SFG) spectroscopy, a resonant IR and a non-resonant visible laser pulse are applied to a sample, and a signal is detected at the sum frequency of the pulses. This signal is sensitive to the local environments of interfacial chromophores. For the *psp* polarization combination (*p*-polarized SF, *s*-polarized visible, *p*-polarized IR), the signal is selectively sensitive to chiral structures. Recently, it was found that peptide secondary structures could be distinguished by the presence or absence of *psp* signals for the amide I and NH stretch modes. This finding has been exploited to track the aggregation of human islet amyloid polypeptide at a water/air interface. To facilitate the interpretation of these experiments in terms of detailed structures, we present here a mixed quantum/classical method for the computation of both achiral and chiral SFG spectra for the peptide amide I mode, based on classical molecular dynamics simulations. We then apply this method to model systems, and comment as to the importance of both intrinsic chirality (the presence of atomic chiral centers) and structural chirality (the presence of chiral secondary structure) to the strength of the *psp* signal.

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