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Non-adiabatic vibrational-electronic resonance in a model dimer - Implications for Photosynthetic Energy Transfer[1] VIVEK TIWARI, DAVID JONAS, Univ of Colorado - Boulder — Recently Tiwari et al. [PNAS (2013)] have shown that for a model donor-acceptor system resonance between a vibrational quantum of energy of a weakly coupled Franck-Condon vibration and the excited state excitonic energy gap leads to an unavoidable nested energy funnel on the excited state of photosynthetic antennas. Anti-correlated nuclear motions on the two pigments are responsible for such non-adiabatic effects. Here we show that several vibrational modes lying close to an excitonic energy gap in the FMO antenna complex, and a finite width of vibrational-electronic resonance lead to an even stronger non-adiabatic vibrational-electronic mixing along a generalized energy tuning coordinate. Such a generalized tuning coordinate is similar to the "tuning coordinate" in a conical intersection. The 2D spectroscopic signatures of the resulting non-adiabatic effects are additive and lead to more than 2x enhancement of ground state anti-correlated vibrational wavepackets which are expected to dominate the long-lived 2D signatures. Thus, several near-resonant vibrations and a finite width of non-adiabatic coupling render the nested energy funnel in the FMO antenna as a robust and promising design principle for artificial energy and charge transport.

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