2D IR SPECTROSCOPY OF ORGANIC PHOTOVOLTAIC MATERIALS

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Two-dimensional infrared vibrational spectroscopy is used to examine conformational inhomogeneity and ultrafast orientational motion within local environments of an organic photovoltaic (OPV) material. The OPV material consists of a mixture of the electron donor CN-MEH-PPV and the electron acceptor PCBM. PCBM species reside in a distribution of environments within large domains of the molecules that cause their C=O stretch modes to be inhomogeneously broadened. The butyric acid methyl ester group of PCBM undergoes ultrafast wobbling-in-the-cone orientational motion on the 110 fs time scale within a cone semiangle of 29 degrees. The vibrational dynamics are sensitive metrics of molecular order in the organic photovoltaic material.