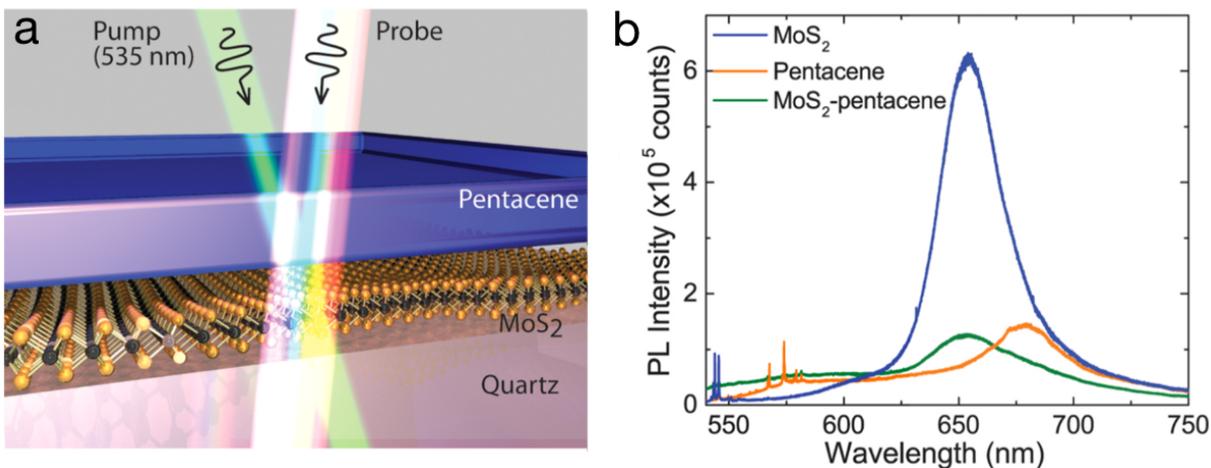


## Ultrafast Exciton Dissociation and Long-Lived Charge Separation in a Photovoltaic Pentacene-MoS<sub>2</sub> van der Waals heterojunction.

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**Caption:** (a) Schematic depiction of the vertical pentacene-monolayer MoS<sub>2</sub> p-n heterojunction being probed by transient absorption spectroscopy. (b) Photoluminescence spectroscopy of the pentacene-MoS<sub>2</sub> heterojunction and its constituent materials, showing quenched MoS<sub>2</sub> photoluminescence in the type-II heterojunction.

### Scientific Achievement

Using transient absorption spectroscopy (TAS), **Hersam** characterized the dynamics of charge transfer in a prototypical type-II vertical organic molecular-2D TMD heterojunction of pentacene, a p-type molecular donor, and monolayer MoS<sub>2</sub>, an n-type 2D acceptor. TAS revealed the timescales of photo-excited carrier dynamics, including hole charge transfer occurring in 6.7 picoseconds, radiative recombination in 431 picoseconds, and charge recombination in ~5 nanoseconds. As a result, the overall hole transfer yield is ~50%, such that hole transfer is fast enough to outcompete all hole relaxation processes except sub-picosecond carrier trapping, as is desirable for optoelectronic applications such as photovoltaics.

### Significance

The realization of ultrathin p-n heterojunctions has potential applications in a range of electronic and optoelectronic devices including anti-ambipolar transistors and mechanically flexible photovoltaics. However, doping of the constituent 2D materials remains a challenge. While conventional substitutional doping is possible for 2D materials, this method tends to increase charge carrier scattering and limit electronic properties. In contrast, charge transfer from surface adlayers allows for doping of 2D semiconductors without introducing structural defects to the 2D

crystal. In this study, the charge transfer dynamics of a vertical pentacene-2D MoS<sub>2</sub> p-n heterojunction have been elucidated, demonstrating ultrafast charge transfer and long carrier lifetimes. Due to the large degree of tunability in the structure and properties of 2D semiconductors and organic adlayers, this approach can be generalized to a wide variety of heterojunctions, thereby enabling diverse applications in electronics and optoelectronics.

**Citation**

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