2DCC MIP at Penn State, DMR-1539916

External User Project - 2021

Ultrafast optical melting of trimer superstructure in layered 1T′-TaTe2

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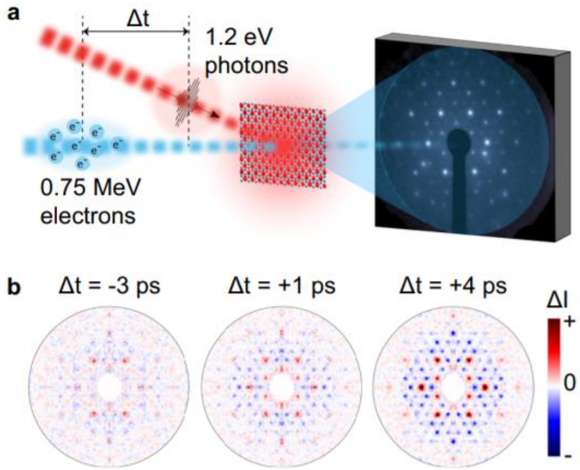
Project Summary: Quasi-two-dimensional transition-metal dichalcogenides are a key platform for exploring emergent nanoscale phenomena arising from complex interactions. Access to the underlying degrees-of-freedom on their natural time scales motivates the use of advanced ultrafast probes sensitive to self-organized atomic-scale patterns. The Kaindl group at Lawrence Berkeley National Lab recently reported the ultrafast investigation of 1T'-$TaTe_2$, demonstrating a rapid picosecond melting of its trimer cluster lattice superstructure in the low temperature (LT) phase. They observed photo-induced melting of the LT order on 1.4 ps timescale, indicative of fast switching, followed by recovery into a hot (3 × 3) trimer phase. Insight into the nature of trimer cluster melting is obtained via density functional calculations, which indicate an initial quench driven by charge-transfer transitions from bonding to non-bonding states of the Ta trimer—suggesting pathways for a photo-induced transition that is unique among the family of TaX_2 materials. This work establishes $TaTe_2$ as a promising material for optical control, motivating examination of concomitant electronic dynamics for device applications. Published in *Communications Physics* 4, 152 (2021).

2DCC Role: This research resulted from the collaboration between a 2DCC external user, Prof. Kaindl at Lawrence Berkeley National Laboratory, and the researchers of the 2DCC Bulk Growth team. The single crystals of 1T'-$TaTe_2$ used for this study were grown using a chemical vapor transport method at the 2DCC Bulk Growth facility.



(a) Illustration of the optical pump, electron diffraction probe experiment. (b) Photo-induced changes in the diffraction patterns, for selected time delays. The colour scale gives the absolute diffracted intensity change (ΔI).