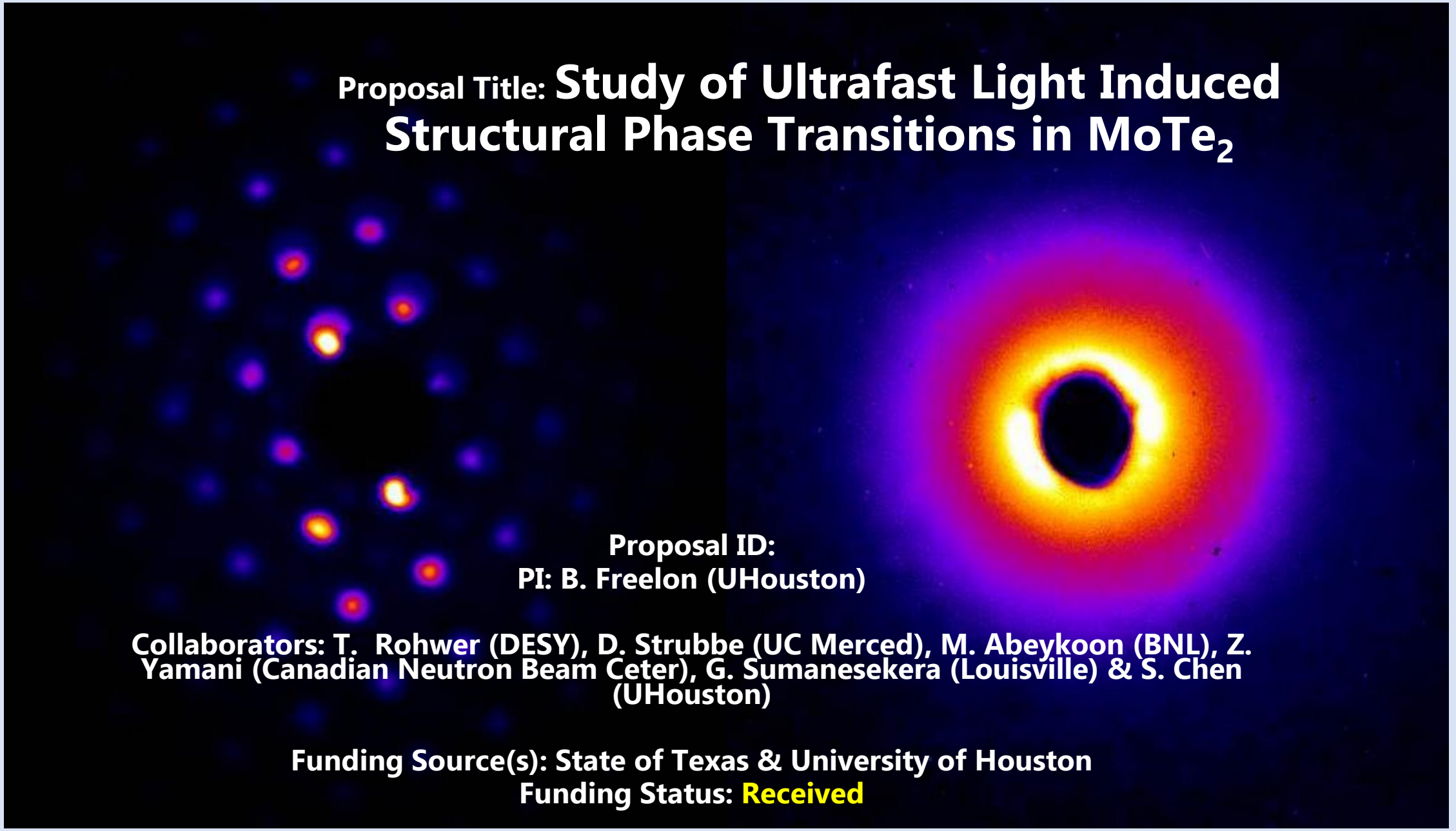


Proposal Title: **Study of Ultrafast Light Induced Structural Phase Transitions in $MoTe_2$**

Proposal ID:

PI: B. Freelon (UHouston)

Collaborators: T. Rohwer (DESY), D. Strubbe (UC Merced), M. Abeykoon (BNL), Z. Yamani (Canadian Neutron Beam Ceter), G. Sumanesekera (Louisville) & S. Chen (UHouston)

Funding Source(s): State of Texas & University of Houston

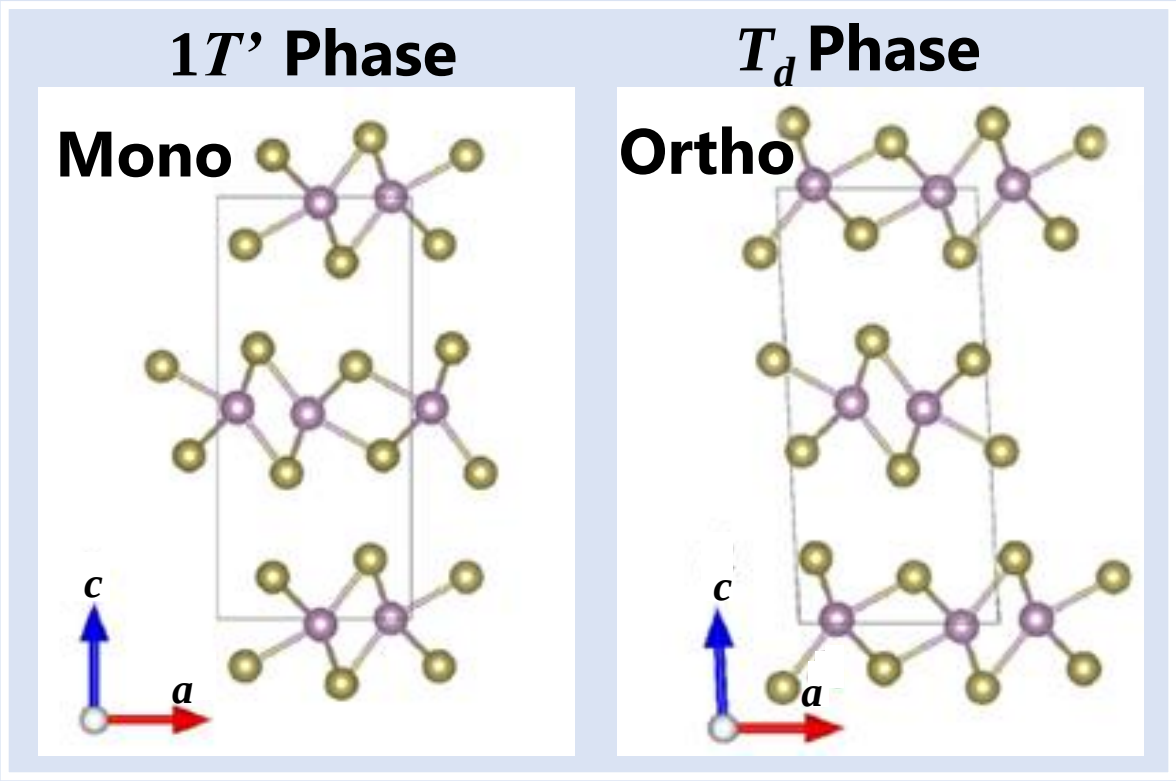
Funding Status: Received

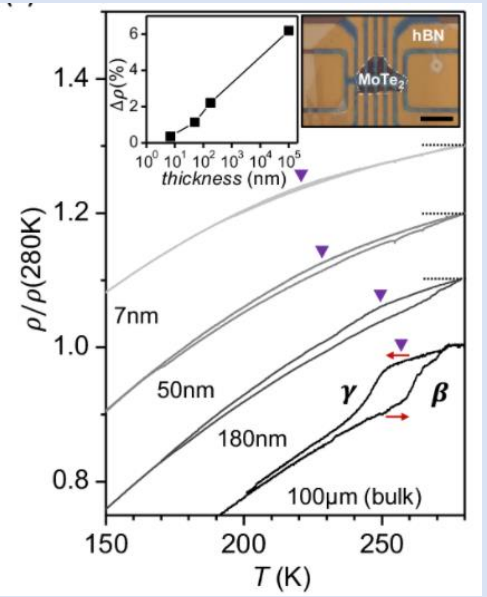
Transition Metal Dichalcogenide $MoTe_2$

- 2D van der Waals crystal
- Weyl fermions emerge at the boundary of electron/hole pockets
- Topologically non-trivial band structure & superconductivity
- Proposed to be a topological switch material: thermal and photonic
- $1T'$ semiconducting phase to T_d phase topological Weyl semi-metallic phase
- The low temperature T_d state exhibits
  - Very large magnetoresistance
  - Superconductivity with possible unconventional origins
  - Type-II Weyl nodes
  - Broken inversion symmetry phase.

1T'-MoTe2

- $1T$'-$MoTe_2$ is a structurally stable but delicate material
- The 1T' to T_d structural phase transition (SPT) is not well understood
  - Symmetry determination is a challenge
  - 1-st order, coexistence phase region
  - Disorder: stacking faults
  - Dimensionality influences the SPT
- Can we investigate the SPT the evolution from 1T' to T_d using time-resolved methods?

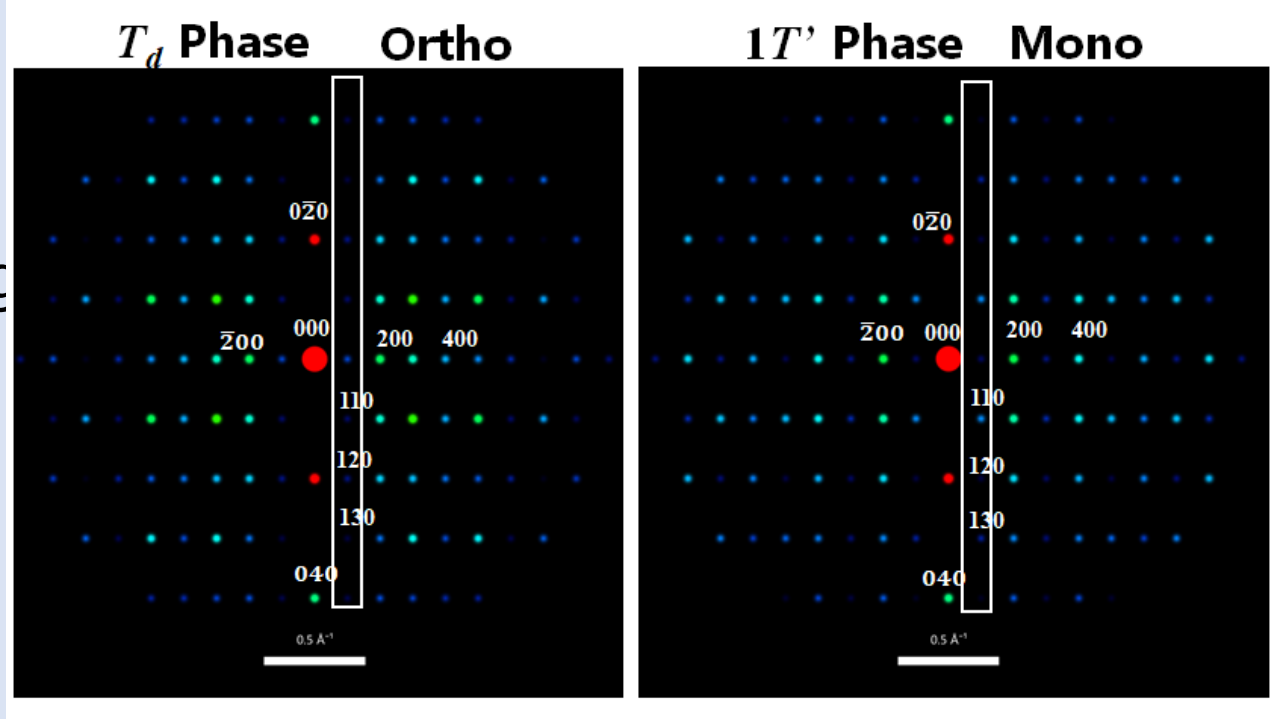




Phys. Rev. B **97**, 041410(R) (2018)

1T'-MoTe2

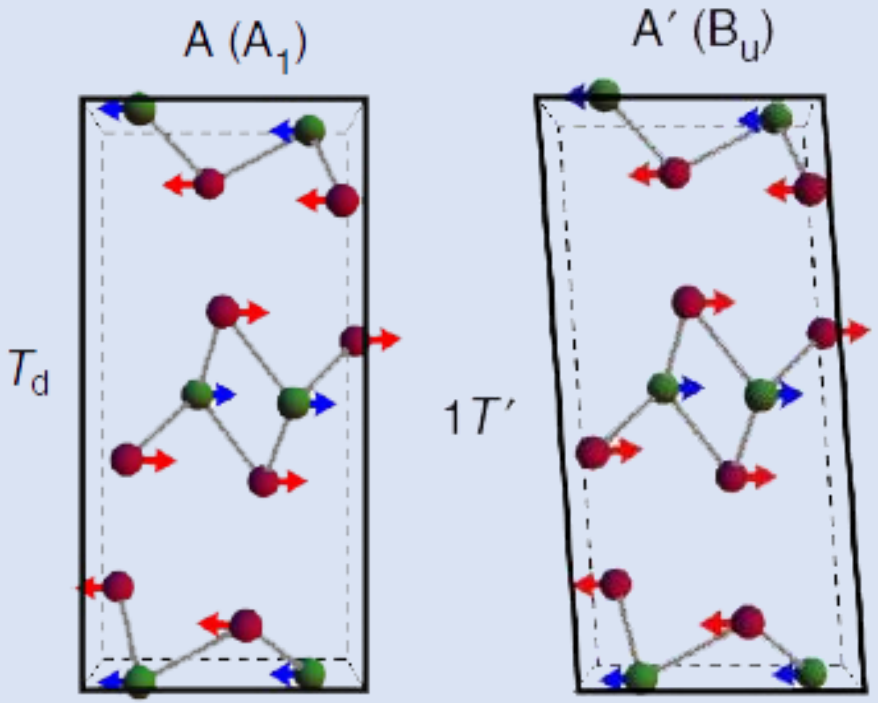
- 1T' to T_d SPT near 250K
- Large co-existence region 1T' + T_d
- Static diffraction complicated by stacking faults
- Appearance of a new phase T*
- Average structure (Bragg diffraction) can detect SPT-related symmetry changes
  - Overlooks local structural changes that might drive subtle transformations (from 1T' to T_d)
- SPT behavior growth & dimension-dependent



Simulated Electron Diffraction of $MoTe_2$

Photo-induced SPT in $1T'$-MoTe2

- 800 nm ultrafast light can drive the $1T'$ to T_d SPT under sufficient pump fluences
- Use the appearance of shear-mode Raman modes to identify the $1T'$ to T_d SPT
  - A-mode invisible in the $1T'$-phase
- Track the (*hk0*) Bragg peaks with different non-zero *k* values to track the sliding of the layers in the non-equilibrium state
- Can we investigate the structural phase transition: the evolution from $1T'$ to T_d

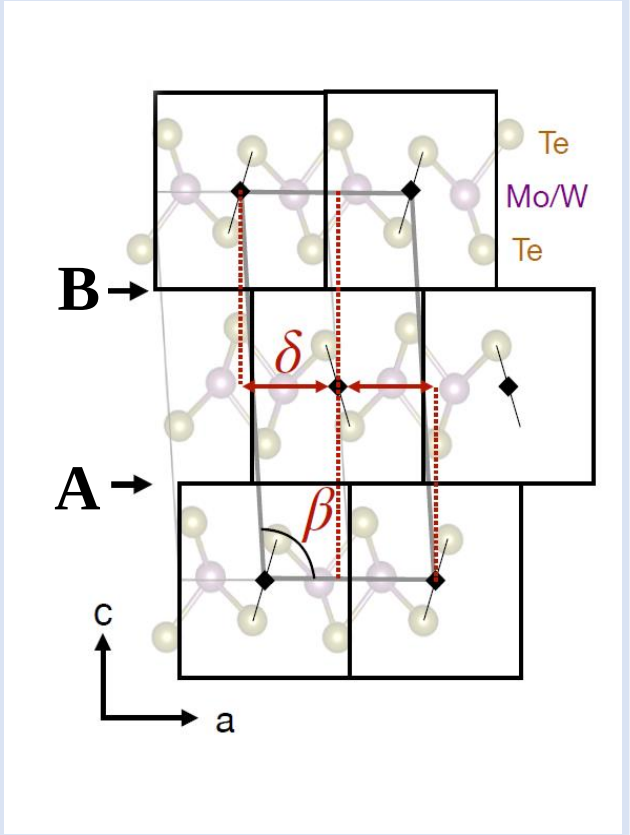


Nat. Comm. **7**, 13552 (2016).

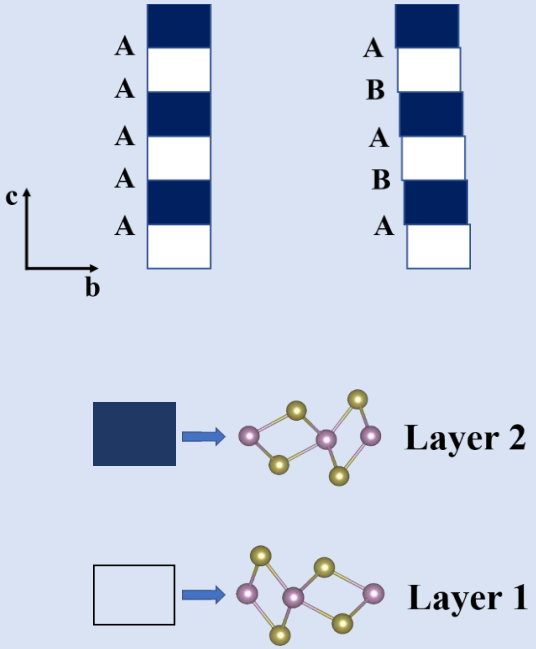
Calculated Raman modes sensitive to the inversion symmetry breaking

Exploring the $1T'$-T_d Transition: Layering

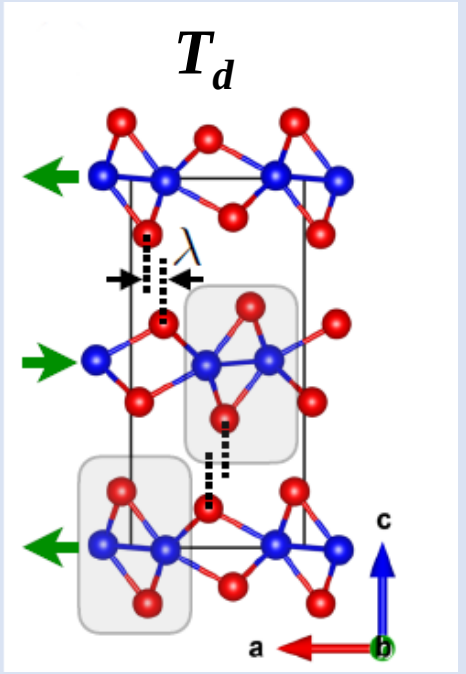
- $1T'$ to T_d SPT can be viewed as layer sequencing process
- Layer models
  - 2 layer structures
  - Sequences of 2 transitions A an B
  - Reproduces the $1T'$ and T_d phases



Layer Sequencing Model

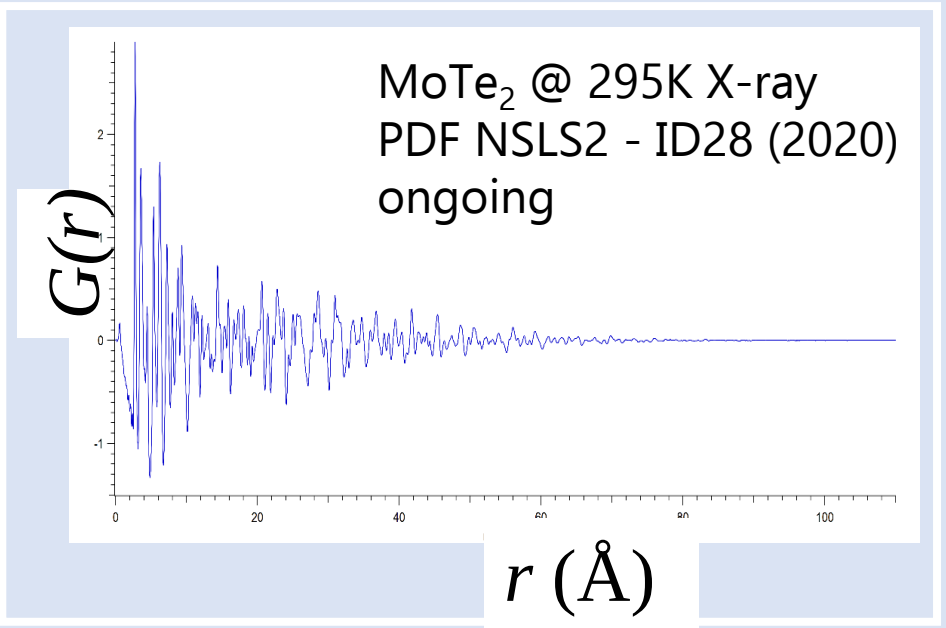


$1T'$-T_d Phase Transition: Local Ordering



- Investigate the use of electron Pair Distribution Function (ePDF) technique
- Interlayer sliding: subtle local changes to expose the $1T'$-T_d evolution
- λ-parameter determination
- Large box modelling (RMCprofile), Molecular Dynamics, DFT) to track these parameters in the non-equilibrium state

- Establish Proof-of-principle?
  - Determine sufficient PDF peak intensity
  - Confirm PDF fit-worthiness at high energy (MeV): compression of scattering peaks



Special Equipment Requirements & Hazards

- User Sample and Setup
  - Please indicate any special equipment that you expect to need bolometer/interferometer setup etc: **NO**
- Pump Laser Requirements
  - Please note any special pump laser requirements here: **NO**
- Hazards & Special Installation Requirements
  - Large installation (chamber, insertion device, etc.): **NO**
  - Cryogens: (liquid Nitrogen) **YES**
  - Introducing new magnetic elements: **NO**
  - Introducing new materials into the beam path: **YES**
  - Any other foreseeable beam line modifications: **NO**

Experimental Time Request

CY2021 Time Request

Capability	Setup Hours	Running Hours
UED Facility	60	300

Time Estimate for Full 3-year Experiment (including CY2020)

Capability	Setup Hours	Running Hours
UED Facility	100	600