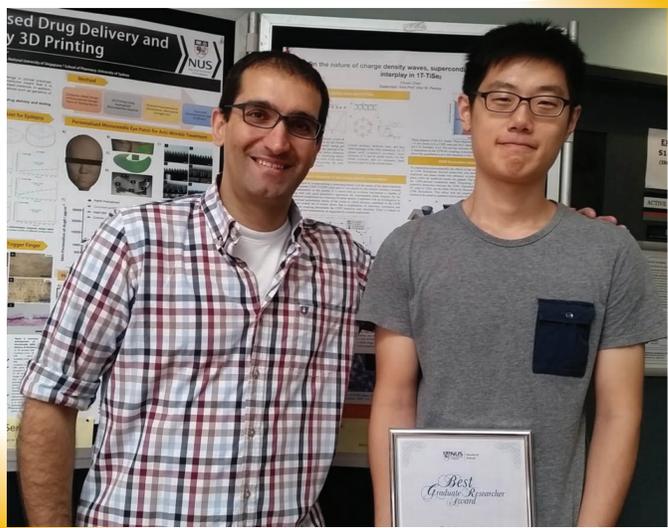


# Chen Chuan



Chen Chuan with his supervisor, Assistant Professor Vitor Manuel Pereira

## Achievements

Throughout his PhD in Physics, Chuan developed an original body of theoretical work that provides the most comprehensive and detailed investigation to date of the charge-density wave (CDW) instability in TiSe<sub>2</sub>, its microscopic underpinnings as an excitonic condensation instability, and how CDW fluctuations might be essential to explain the experimental observation of superconductivity in this compound at low temperatures.

His work is reported in a series of 4 research papers, the first of which (published in Physical Review Letters) establishes the crucial role of the excitonic instability, possibly settling a question that has endured 40 years of polarizing discussions in the literature and the community.

The momentum gained in this first paper has been fruitfully directed to building a comprehensive theoretical picture of not only CDW physics, but also how the CDW order might be responsible for the emergence of superconductivity with doping in TiSe<sub>2</sub>. Unlike the CDW problem that has a long history, the nature of the superconductivity in this system is a new and entirely unexplored topic. Chuan's subsequent work contributes the first theory that reproduces the whole phase diagram. In his second paper nearly ready for submission, he establishes how the two order parameters must be coupled at the level of a Ginzburg-Landau theory in order to explain the experiments; he furthermore predicts that superconductivity is likely to be spatially inhomogeneous and strongly associated with CDW discommensurations, which agrees with recent experimental suggestions. His third paper is the necessary follow-up that goes back to the microscopic Hamiltonian and demonstrates that fluctuations of CDW order can induce superconducting pairing. The implication is that thermal and quantum fluctuations of the excitonic state he established with his first paper are the likely microscopic origin of the superconducting dome observed experimentally. Fluctuation-induced pairing has deep connections with models that explain the high-temperature superconductivity in cuprate oxides.

Finally, in collaboration with an experimental group at NUS, Chuan contributed theory to interpret and understand the superconducting phase diagram of strictly two-dimensional TiSe<sub>2</sub>, in which magneto-transport measurements reveal a quantum phase transition from superconducting to a Bose-metallic phase. The latter has been observed recently in a number of two-dimensional superconductors and is a new challenge in our understanding of the superconducting ground state in two-dimensions.

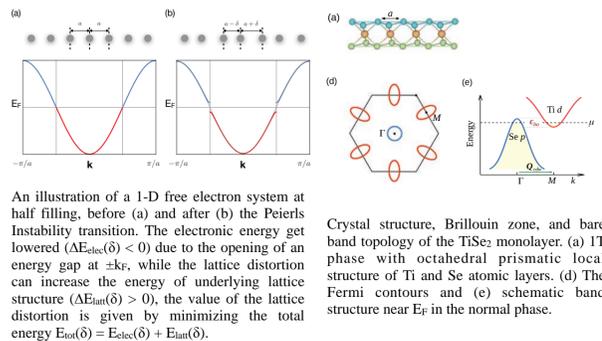
## Publications

- [1] C. Chen, B. Singh, H. Lin, Vitor M. Pereira, "Reproduction of the Charge Density Wave Phase Diagram in 1T-TiSe<sub>2</sub> Exposes its Excitonic Character". Phys. Rev. Lett. 121, 226602 (2018).
- [2] C. Chen, L. Su, A. H. Castro Neto, Vitor M. Pereira, "Discommensuration-enhanced superconductivity in the charge density wave phases of transition-metal dichalcogenides". Submitted. arXiv:1806.08064 (2018).
- [3] C. Chen, A. H. Castro Neto, Vitor M. Pereira, "Pairing induced by fluctuations of an excitonic insulator: the case of superconductivity in TiSe<sub>2</sub>". In preparation.
- [4] L. Li, C. Chen, et al., "Anomalous quantum metal in a 2D crystalline superconductor with intrinsic electronic non-uniformity". Submitted. arXiv:1803.10936 (2018).

## On the nature of charge density waves, superconductivity and their interplay in 1T-TiSe<sub>2</sub>

Chuan Chen  
Supervisor: Asst Prof. Vitor M. Pereira

### Charge density wave and 1T-TiSe<sub>2</sub>

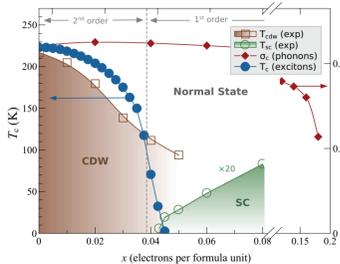


An illustration of a 1-D free electron system at half filling, before (a) and after (b) the Peierls Instability transition. The electronic energy get lowered ( $\Delta E_{elec}(\delta) < 0$ ) due to the opening of an energy gap at  $\pm k_F$ , while the lattice distortion can increase the energy of underlying lattice structure ( $\Delta E_{lat}(\delta) > 0$ ), the value of the lattice distortion is given by minimizing the total energy  $E_{tot}(\delta) = E_{elec}(\delta) + E_{lat}(\delta)$ .

Crystal structure, Brillouin zone, and bare band topology of the TiSe<sub>2</sub> monolayer. (a) 1T phase with octahedral prismatic local structure of Ti and Se atomic layers. (d) The Fermi contours and (e) schematic band structure near  $E_F$  in the normal phase.

### Excitonic character of the charge density wave phase

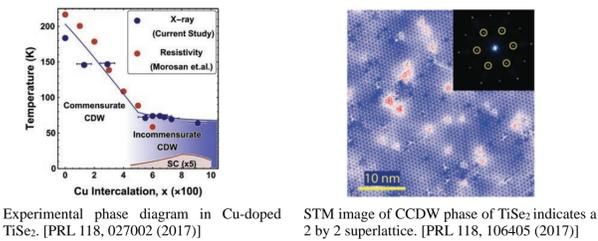
My research begins by re-approaching a years-long debate over the nature of the phase transition to the commensurate CDW (CCDW) state and the role played by the intrinsic tendency towards excitonic condensation in this system. It is shown that an excitonic mechanism is capable of reproducing with very good quantitative agreement the experimental phase diagram for the CCDW transition temperature as a function of carrier density. Combined with an investigation by density functional perturbation theory of the extent to which phonons contribute to the CDW instability, the overall set of results shows that a combination of electronic correlation and electron-phonon coupling precipitates the CDW transition and, therefore, TiSe<sub>2</sub> is indeed an excitonic solid at low temperatures, as suggested by a recent experiment.



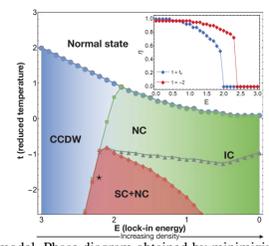
Comparison between experimental and theoretical phase diagrams for the CDW transition in Cu<sub>x</sub>TiSe<sub>2</sub>. The blue circles represent  $T_c$  obtained from the self-consistent solution which includes only the excitonic mechanism. Its reduction with doping follows the experimental trend with very good qualitative and quantitative agreement up to  $x \approx 0.038$ . At this doping, the transition becomes of 1st order in our calculation which approximately coincides with the experimental observation of ICDW signatures and the onset of the SC dome at  $x \approx 0.04$ . The red diamonds show the variation in the critical smearing parameter ( $\alpha_c$ ) above which the dynamical phonon instability disappears in the DFPT calculations.  $\alpha_c$  remains nearly unaltered in the experimentally relevant range of  $x$ , and only drops to zero beyond  $x \approx 0.2$ , suggesting that, without the adequate account of the electronic interactions, the phonon calculation predicts the PLD to be stable up to unrealistically high doping.

### Discommensuration enhanced superconductivity

A Ginzburg-Landau phenomenological theory was subsequently developed to understand the experimentally observed transition from commensurate to incommensurate CDW (ICDW) order with doping or pressure, and the emergence of a superconducting dome that coexists with ICDW. By phenomenologically mapping the lock-in energy to the carrier density, one obtains results and a phase diagram where: (i) the CCDW is suppressed and evolves into ICDW with doping or pressure, (ii) SC can coexist with ICDW at low temperatures and a finite range of densities, (iii) SC order first arises within the CDW discommensurations at the near-commensurate transition. These results are in line with the experimental phase diagram.



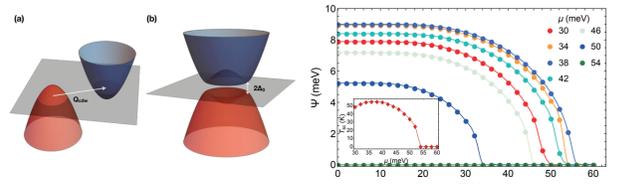
Experimental phase diagram in Cu-doped TiSe<sub>2</sub>. [PRL 118, 027002 (2017)] STM image of CCDW phase of TiSe<sub>2</sub> indicates a 2 by 2 superlattice. [PRL 118, 106405 (2017)]



Phase diagram of the G-L model. Phase diagram obtained by minimizing free energy. When  $F_{CDW} < 0$ , the system is in a CDW state and the C phase corresponds to  $\eta = 0$ . The green line represents the C-IC boundary,  $E_c(\eta)$ . The red line indicates the boundary of the SC phase including the linear E dependence in the CDW-SC coupling; it becomes the gray line if as is E-independent. The inset shows the equilibrium  $\eta$  at  $T_c$  (the transition is first order) and at low temperature.

### CDW fluctuation induced superconductivity

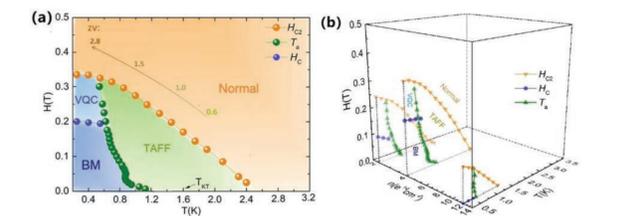
To characterize microscopically the effects of the interplay between CDW and SC, the spectrum of CDW fluctuations beyond mean-field was studied in detail. The effective action for the amplitude and phase modes was obtained, revealing the gapless (Goldstone) character of the phase while the amplitude modes are gapped. The addition of charge carriers to the system fills the CDW-dressed conduction band. Integrating CDW fluctuations out leads to a retarded attractive interaction between the CDW "renormalized" quasiparticles. The result indicates that SC order in TiSe<sub>2</sub> can be either driven by fluctuation-induced pairing or, at least, enhanced by CDW fluctuations. This tallies with the experimental observation that the SC dome appears centered at the putative quantum critical point of the CCDW phase.



Band structure of simplified model. (a) The "bare" band structure of the simplified model, which consists of a hole-like valence band (red) and an electron-like conduction band (blue). The two bands are perfectly nested to each other with a nesting wavevector  $Q_{nest}$ . (b) The mean field potential/doping level. As the chemical potential "renormalized" band. The gap between conduction and valence band is  $2\Delta_0$ , with  $\Delta_0$  being the mean field value of CDW order parameter.

### Anomalous quantum metal in 1T-TiSe<sub>2</sub>

Collaborating with experimental groups, we discovered that with increasing magnetic field, an anomalous quantum metal (AQM) phase emerges between the SC to normal metal transition. A scaling analysis about the resistance suggests that within the AQM phase, there is a crossover from a low field Bose metal regime to a high field vortex quantum creeping regime. Since the onset of SC behavior in TiSe<sub>2</sub> coincides with the disruption of commensurate CDW order through discommensurations, we advance that the development of the SC order parameter is inescapably intertwined with that of the charge density and its fluctuations. This has a direct implication in terms of providing both an intrinsic spatial non-uniformity for the development of the AQM, as well as a natural dissipation channel via phase fluctuations of the CDW.



Phase diagram of two-dimensional superconducting 1T-TiSe<sub>2</sub>. (a) The field-temperature phase diagram when the carrier density is tuned to  $n = 4.0 \times 10^{14} \text{ cm}^{-2}$ . Thermally assisted flux flow (TAFF) exists between the lines labeled  $H_{c2}(T)$  and  $T_{c2}(H)$  while the anomalous quantum metal (AQM) is observed below the  $T_{c2}(H)$  line. The scaling exponent  $z\nu$  obtained for different temperature ranges is also indicated. Its systematic increase from the clean to quantum percolation regimes with decreasing temperature is indicative of spatial inhomogeneity likely attributed to the underlying CDW order, and the dominant role of quantum fluctuations at the lowest temperatures. (b) Phase diagram extended along the density axis summarizing the transport behaviour for the under- and over-doped cases. The AQM is prevalent as  $T \rightarrow 0$ , and the different regimes have a dome-like dependence on carrier density.

References:  
[1]. arXiv: 1712.04967v1; [2]. arXiv: 1806.08064; [3]. arXiv: 1803.10936



Department of Physics  
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## Research Areas

The core of Chuan's research is dedicated to the theoretical understanding of effects arising from electronic interactions and the interplay between different microscopic degrees of freedom (including disorder) in so-called strongly-correlated systems. He has focused, in particular, in the microscopic interplay between charge density waves (CDW) and superconductivity (SC) in either layered 3D or strictly 2D crystals.

Generically, the interplay of CDW and SC orders is one of the perennial topics of interest in condensed matter physics because there are specific reasons to believe that progress in characterizing the underlying physics can unlock many of the unresolved problems in high-temperature superconductivity, where competition among spin or charge order and SC are also present. Transitions among these phases are usually driven by temperature or electronic doping. Research on these correlated ground states has been explosively revived over the last 5 years with the possibility of exploring them in a number of different 2D realizations of layered crystals, because of the ability of tuning the carrier density on demand by field effect, without introducing disorder. This is currently one of the hottest topics in experimental and theoretical condensed matter research, as documented by the pace of high-profile publications appearing in Science and Nature-branded journals during 2016-2018.



Chen Chuan receiving his award from Prof Lu Yixin, Vice Dean (Graduate Studies and Safety)

## Awards

- ✓ 2018- Best Graduate Researcher Award (Physics). Faculty of Science, NUS.
- ✓ 2013- 1st Class Scholarship of National Scientific Base for Talented Persons 2013-2014. Sichuan University.
- ✓ 2012- 1st Class Scholarship of National Scientific Base for Talented Persons 2012-2013. Sichuan University.
- ✓ 2011- National Scholarship 2011-2012. Sichuan University.
- ✓ 2010- National Scholarship 2010-2011. Sichuan University.