Electronic properties of 1T–$TiSe_2$, numerical models of the formulation and melting of the charge density wave state

J. A. Gray, J. S. Smith and J. H. Cole

Chemical and Quantum Physics, and ARC Centre for Excellence in Future Low-Energy Electronics Technologies, School of Science, RMIT University, Melbourne, Victoria 3000, Australia.

The charge density wave (CDW) is an example of a low temperature phase of matter which occurs due to strongly correlated electrons. CDW materials are characterised by a periodic distortion of the atomic lattice, periodic modulation of the electronic charge distribution, and a complex order parameter. These materials have potential application in mechanical vibration detectors, optoelectric devices, information processing, memory, and many other next generation technologies. Many strongly correlated materials show non-trivial phases at similar temperatures and energy scales, and because of this, disentangling the mechanisms behind the phases has historically proven difficult using standard many-body methods. Here we use dynamical mean-field theory (DMFT) [1] in conjunction with density functional theory (DFT) and time-dependent Ginzburg–Landau (TDGL) formalism [2] to investigate the electronic properties of the CDW material 1T–$TiSe_2$. Using these numerical techniques, we can understand both the formation of the CDW state and the melting of this phase due to the application of laser pulses and the resulting heating of the phononic environment.

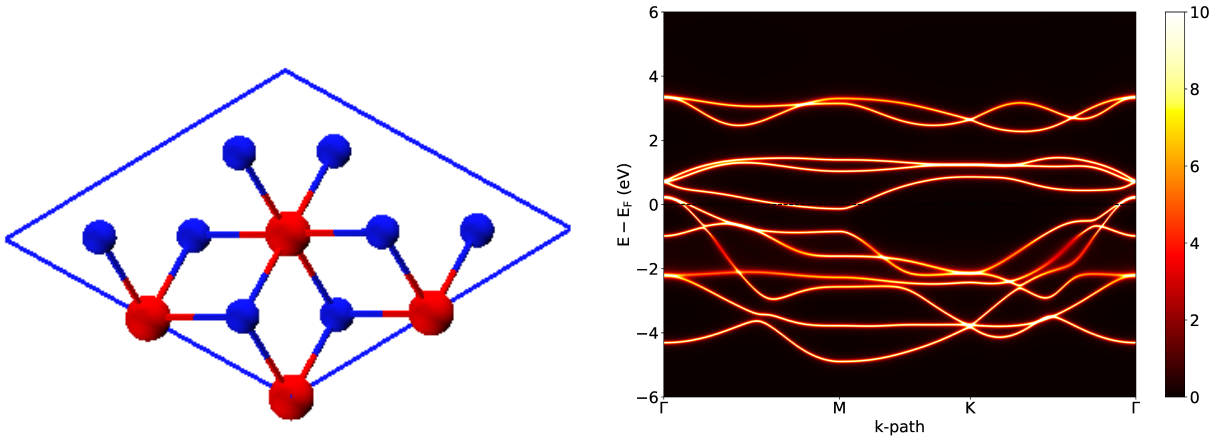

Figure 1: Supercell for the 2x2 structure of undistorted, intrinsic, single layer 1T–$TiSe_2$ (left) showing Ti (red) and Se (blue) atomic positions, and the calculated DMFT spectral function for this structure (right).

[1] V. Singh *et al*, *Comput. Phys. Commun.* **261**, p. 107778 (2021).

[2] P. E. Dolgirev *et al*, *Phys. Rev. B.* **101**, p. 054203 (2020).