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Correlations and dimerization in the domain walls of triangular-lattice Mott insulator 1T-TaS2

1T-TaS2 is a charge-density-wave (CDW) compound with a Mott-insulating ground state. The metallic state obtained by doping, substitution or pulsed charge injection is characterized by an emergent CDW domain wall network, while single domain walls can be found in the pristine Mott state. Tunneling spectroscopy reveals partial suppression of the Mott gap and the presence of in-gap states strongly localized at the domain-wall sites. Using the real-space dynamical mean field theory description of the strongly correlated quantum-paramagnet ground state I will show that the local gap suppression follows from the increased hopping along the connected zig-zag chain of lattice sites forming the domain wall, and that full metallisation is preempted by the splitting of the quasiparticle band into bonding and antibonding sub-bands due to the structural dimerization of the wall, explaining the presence of the in-gap states and the low density of states at the Fermi level.