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Zigzag-chain domain walls facilitate metalisation of the Mott insulator on a triangular lattice

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We consider the Hubbard model on a triangular lattice as a low-energy effective model describing the narrow electron band formed around the Fermi level in the low-temperature commensurate $\sqrt{13} \times \sqrt{13}$ charge-density-wave (CDW) phase of 1T-TaS_2. The triangular superlattice is formed by 13 Ta atoms that undergo displacement toward the central site in the shape of David-star (hexagram). The narrow band undergoes the Mott metal-insulator transition giving rise to the insulating behavior characteristic of this system in its pristine condition. Motivated by the occurrence of a long-lived metastable metallic hidden-state in 1T-TaS_2 that can be induced by optical or voltage pulses and that shows a characteristic mosaic pattern of mesoscale CDW domains separated by a dense web of domain walls, we study in this work how the structural domain walls affect the electron dynamics. In the effective Hubbard model a domain wall between two CDW domains leads to a local modification of the hopping constants along a one-dimensional defect line. We study the resulting Hamiltonian using the extension of the dynamical mean-field theory to inhomogeneous systems. We discuss in detail the case where the hopping constants are enhanced and the domain wall metallises. We show that this is facilitated by the fact that in the triangular lattice the domain walls tend to enhance the hopping constants along a connected zigzag line, rather than forming a ladder of dimers which instead show a band gap. We also discuss the case of multiple domain walls and comment on the relevance of the domain-wall-metallisation scenario for the metallic hidden-state.