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Resolving the chicken-and-egg problem in VO_2: a new paradigm for the Mott transition[1] OSCAR NAJERA, MARCELLO CIVELLI, Laboratoire de Physique des Solides, CNRS-UMR8502, Universite Paris-Sud, Orsay 91405, France, VLADIMIR DOBROSAVLJEVI, Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32306, USA, MARCELO ROZENBERG, Laboratoire de Physique des Solides, CNRS-UMR8502, Universite Paris-Sud, Orsay 91405, France — We consider a minimal model to investigate the metal-insulator transition in VO_2. We adopt a Hubbard model with two orbital per unit cell, which captures the competition between Mott and singlet-dimer localization. We solve the model within Dynamical Mean Field Theory, characterizing in detail the metal-insulator transition and finding new features in the electronic states. We compare our results with available experimental data obtaining good agreement in the relevant model parameter range. Crucially, we can account for puzzling optical conductivity data obtained within the hysteresis region, which we associate to a novel metallic state characterized by a split heavy quasiparticle band. Our results show that the thermal-driven insulator-to-metal transition in VO_2 is entirely compatible with a Mott electronic mechanism, solving a long standing "chicken-and-egg" debate and calling for further research of "Mottronics" applications of this system.

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