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A Microscopic Model for the Strongly Coupled Electron-Ion System in VO_2[1] TIMOTHY LOVORN, SANJOY SARKER, Department of Physics and Astronomy, University of Alabama — The metal-insulator transition (MIT) in vanadium dioxide (VO_2) near 340 K is accompanied by a structural transition, suggesting strong coupling between electronic and lattice degrees of freedom [1]. To help elucidate this relationship, we construct and analyze a microscopic model in which electrons, described by a tight-binding Hamiltonian, are dynamically coupled to Ising-like ionic degrees of freedom. A mean-field decoupling leads to an interacting two-component (pseudo) spin-1 Ising model describing the ions. An analysis of the minimal ionic model reproduces the observed M1 and M2 dimerized phases and rutile metal phase, occurring in the observed order with increasing temperature. All three transitions are first order, as observed. We further find that both dimerization and correlations play crucial roles in describing the insulating M1 phase. We discuss why dynamical coupling of electrons and ions is key to obtain a full understanding of the phenomenology of VO_2, particularly in the context of the phase coexistence [2] observed near the MIT.

[1] D. Paquet and P. Leroux-Hugon, Phys. Rev. B **22**, 5284 (1980).
[2] M. M. Qazilbash et al., Science **318**, 1750 (2007).

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