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Structural energetics of VO_2 under strain[1] CHANUL KIM, CHRIS MARIANETTI, Columbia Univ, THE MARIANETTI GROUP TEAM — Attaining a proper first-principles description of structural energetics in VO_2 is a necessary condition for fully characterizing the metal-to-insulator transition. Of the existing methods which have been employed for total energies, only DFT+U applied under unorthodox conditions (ie. non-spin-polarized (NSP), with an unreasonably small U) has shown promise. In particular, this DFT+U properly captures the qualitative and quantitative energy difference between the monoclinic (M_1) and rutile (R) phases. We explain why this unorthodox procedure works by studying a minimal model of the structural energetics based on the Peierls-Hubbard model; where the exact solution may be compared to Hartree-Fock, single-site dynamical mean-field theory (DMFT), and cluster DMFT. Furthermore, we use this DFT+U approach to calculate the strain phase diagram at T=0, including the R, M_1, and M_2 phases.

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