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 (i.e. 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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