Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

A minimal model for the structural energetics of VO_2[1] CHANUL KIM, CHRIS MARIANETTI, Columbia Univ, THE MARIANETTI GROUP TEAM — Resolving the structural, magnetic, and electronic structure of VO_2 from the first-principles of quantum mechanics is still a forefront problem despite decades of attention. Hybrid functionals have been shown to qualitatively ruin the structural energetics. While density functional theory (DFT) combined with cluster extensions of dynamical mean-field theory (DMFT) have demonstrated promising results in terms of the electronic properties, structural phase stability has not yet been addressed. In order to capture the basic physics of the structural transition, we propose a minimal model of VO_2 based on the one dimensional Peierls-Hubbard model and parameterize this based on DFT calculations of VO_2. The total energy versus dimerization in the minimal mode is then solved numerically exactly using density matrix renormalization group (DMRG) and compared to the Hartree-Fock solution. We demonstrate that the Hartree-Fock solution exhibits the same pathologies as DFT+U, and spin density functional theory for that matter, while the DMRG solution is consistent with experimental observation. Our results demonstrate the critical role of non-locality in the total energy, and this will need to be accounted for to obtain a complete description of VO_2 from first-principles.

[1]The authors acknowledge support from FAME, one of six centers of STARnet, a Semiconductor Research Corporation program sponsored by MARCO and DARPA.

Chanul Kim
Columbia Univ

Date submitted: 06 Nov 2015 Electronic form version 1.4