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Influence of electro-chemo-mechanical coupling on the metal-insulator transition in VO2 JANAKIRAMAN BALACHANDRAN, PANCHAPAKESAN GANESH, JARON KROGEL, HO NYUNG LEE, PAUL KENT, Oak Ridge National Labaratory, OLLE HEINONEN, Argonne National Labaratory — VO_2 is a strongly correlated electronic system that exhibits polymorphic phases, with different electronic and optical properties. It's a classic example where fine electro-chemo-mechanical coupling between the electronic, spin, lattice and orbital degrees of freedom can be exploited to give rise to new emergent functionalities. The ability to grow thin-films of these materials and control its phases by applying external fields has made this a reality. In this talk we will present computational studies aimed at understanding phase-transitions in VO_2 induced by external mechanical fields. Our studies use wide range of beyond-DFT methods for correlated electronic structures, such as DFT+U, hybrid-DFT etc. and we will compare our results with those from quantum monte carlo (QMC) methods, and also relate them to experimental work. Our findings provide a basis for understanding influence of electro-chemo-mechanical coupling on metal-insulator transition in strongly correlated electronic oxides such as vanadium dioxide. * This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division and also as part of the Computational Materials Sciences Program.

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