"Ab-initio" materials simulations for correlated electron systems with vacancies

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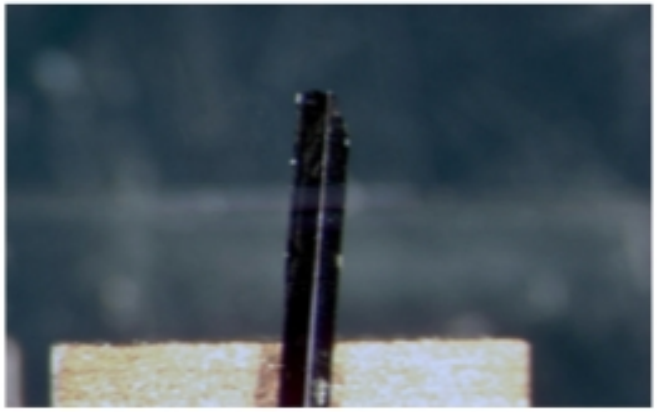
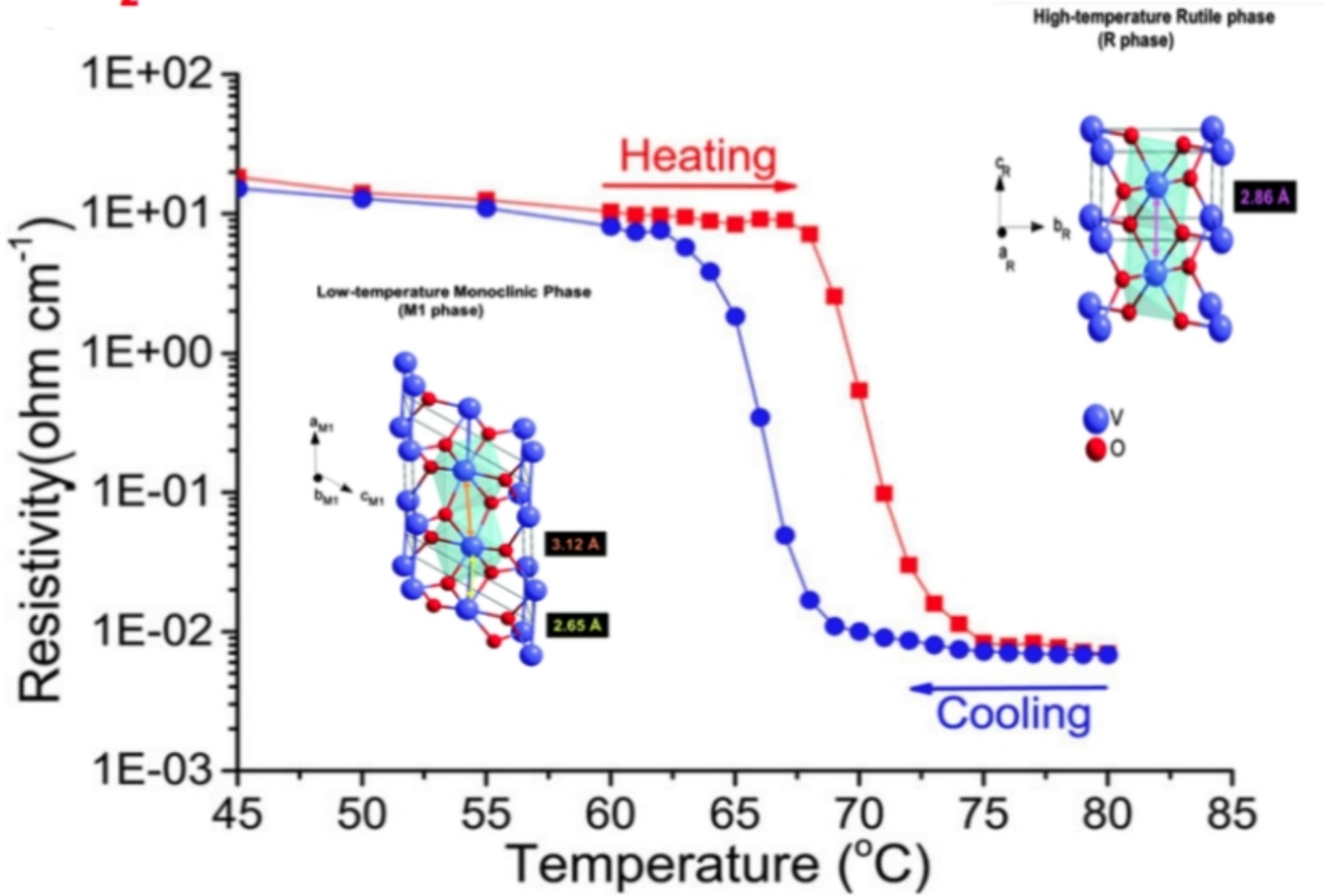


Picture of VO_2 crystal from J. B. Bundai, et al., Nature 515, 535-539 (2014)

VO_2 Metal-Insulator Transition (MIT)



S. Kumer, et al., Nature Scientific Reports, 27699 (2016)

VO_2 Effects of defects on the MIT

DOPING

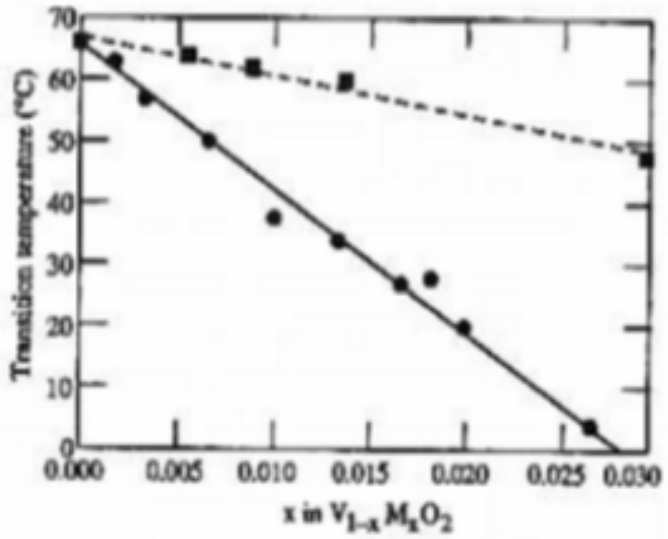
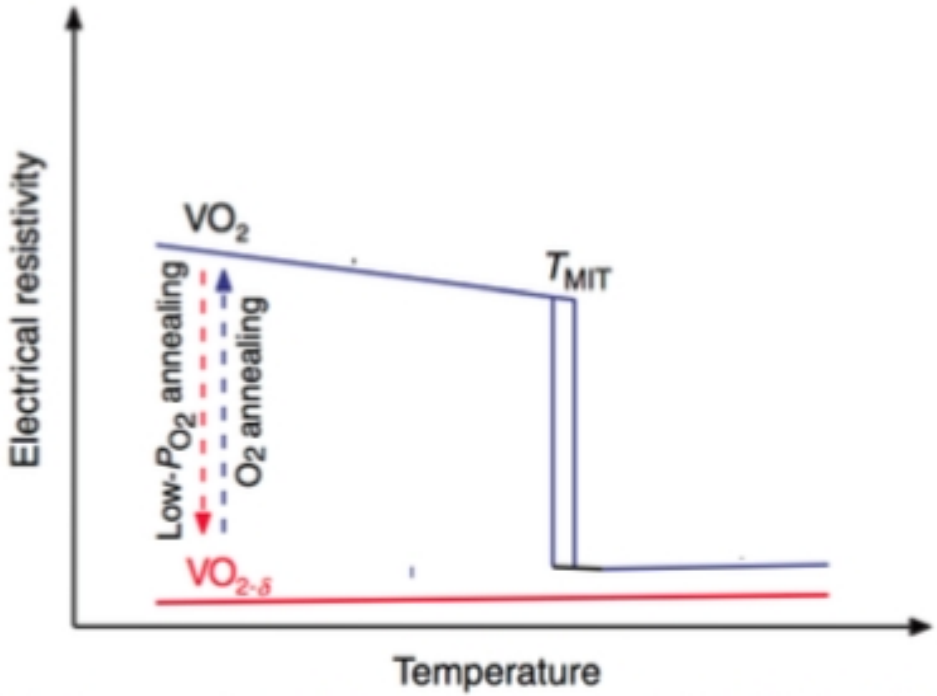


Fig. 3. Monoclinic–tetragonal phase transition temperature $V_{1-x}M_xO_2$ powder where M is (●) tungsten and (■) molybdenum.

. Wei, et al., J. Am. Ceram. Soc. 78, 238-240 (1995)

OXYGEN VACANCIES

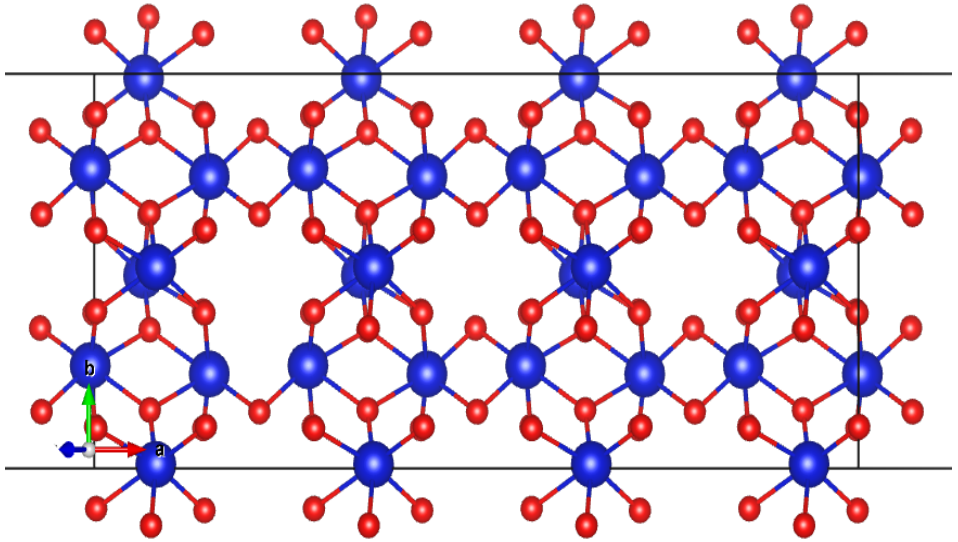


Z. Zheng, et al., Phys. Rev. Apllied 7, 134008 (2017)

Investigation of the nature of the MIT and study of the electronic structure modification due to the presence of defects

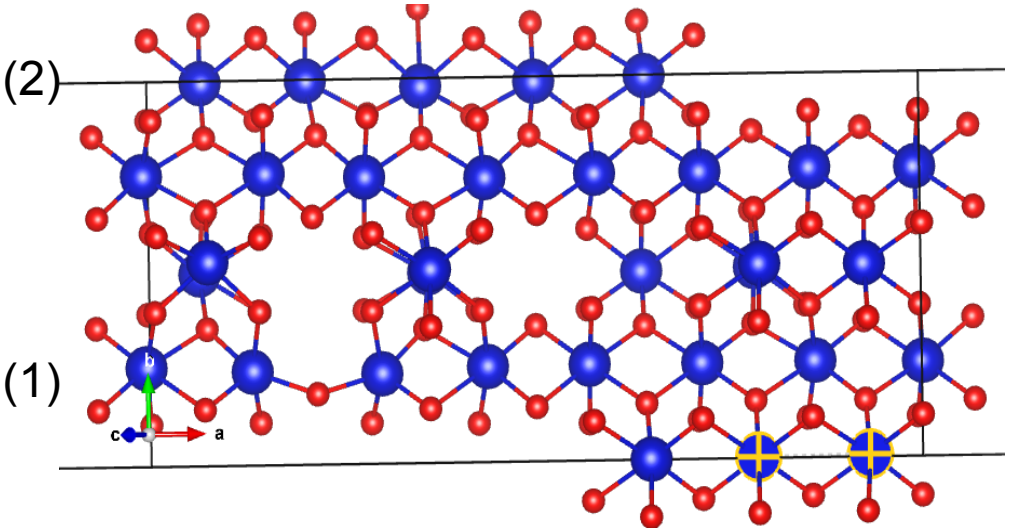
M1 phase with Oxygen vacancies

Unrelaxed (M1 phase)



DA=0.26 A (exp)

Relaxed

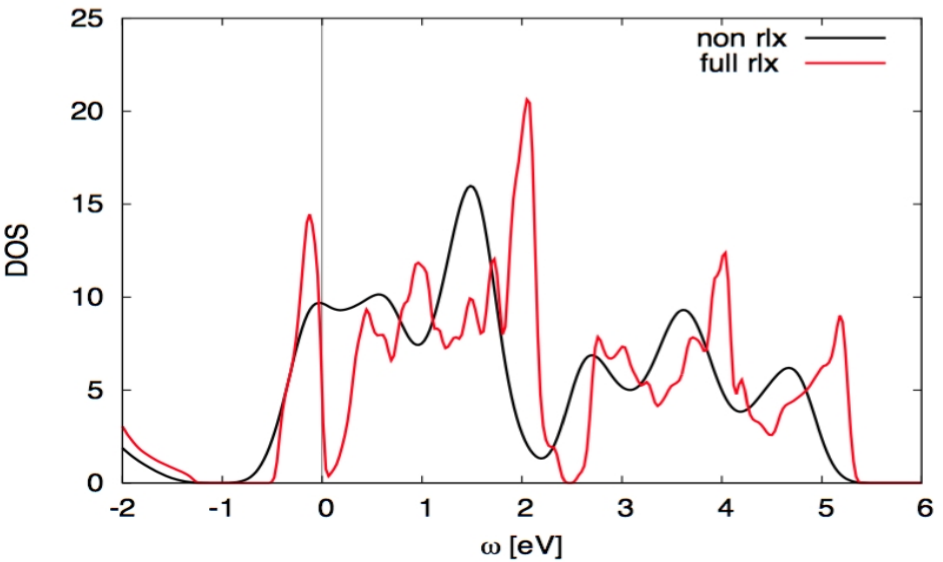


DA=0.16 A (1)
0.06 A (2)

DA =Dimerization amplitude

One missing oxygen atom in a 96 atoms supercell breaks the dimers!

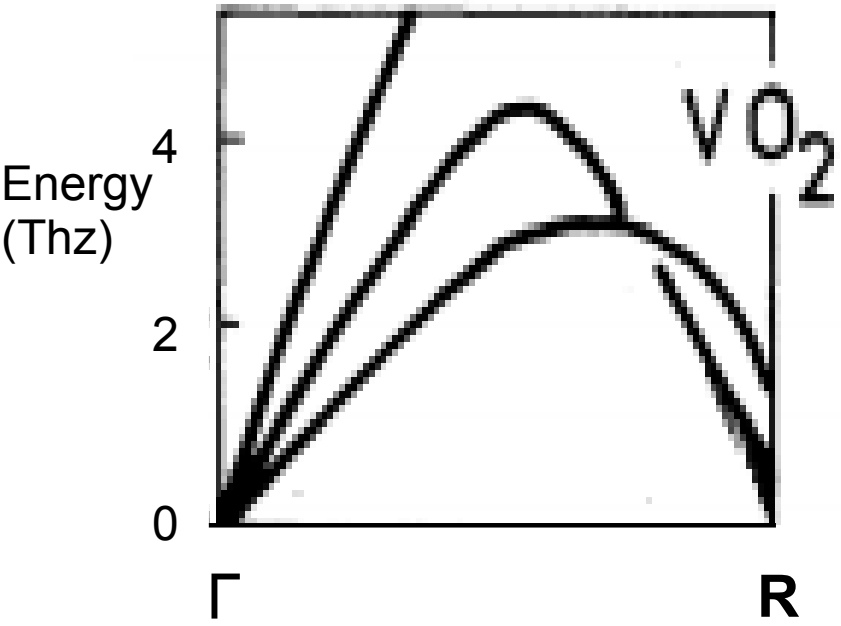
In spite of the fact that Density Functiomal Theory tends to "over-dimerize" the system (DA= 0.35 A)



Phonons

The structural transition can be described in terms of phonons softening

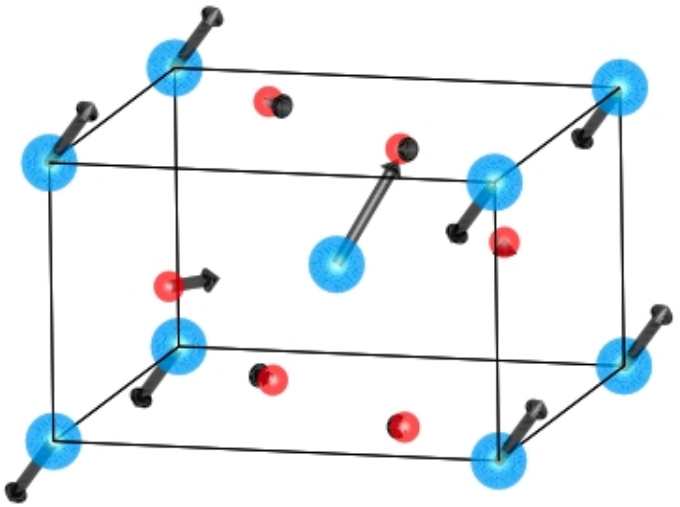
A phonon softening at R point (experimentally observed) resulted from calculations



F Gervais et al., PR B (1985)

Question

How do phonons frequencies depend on doping?



S. Kim et al., PR B (2013)