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**Electrons and phonons in layered and monolayer vanadium pentoxide.<sup>1</sup>**

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Vanadium pentoxide ( $V_2O_5$ ) is a layered material with the potential for interesting new properties when made in 2D mono- or few-layer form. Its band structure is characterized by a split-off conduction band. The lowest conduction band is separated from the rest of the conduction bands by about 1 eV and consists of V- $d_{xy}$  orbitals, non-bonding to the oxygens by symmetry. This narrow band has dispersion essentially along the direction of chains occurring in the layer. When this band becomes half-filled by doping, spin-splitting occurs accompanied by an antiferromagnetic coupling between nearest neighbors along the chain direction. This situation is well known to occur in the so-called ladder compound  $NaV_2O_5$ , which was extensively studied in the late 90s as a potential spin-Peierls or charge ordering compound. However, the monolayer form of  $V_2O_5$  may allow for other ways to control the doping by gating, removing vanadyl oxygens, adsorption of alkali metals, nanoribbon formation, etc. Our calculations predict a switch from antiferromagnetic to ferromagnetic coupling for doping slightly less than half filling of the split-off band. In this talk we will discuss our recent work on the electronic band structure of both bulk and monolayer  $V_2O_5$  as well as the phonons. We find that the quasi-particle self-consistent *GW* method strongly overestimates the band gap. Lattice polarization corrections of the screening are required because of the large LO/TO phonon frequency ratios. Excitonic effects may also be expected to be fairly large. We find that some of the vibrational modes, notably the vanadyl-oxygen bond stretch perpendicular to the layer, unexpectedly shows a strong blue shift. This is explained in terms of reduced screening affecting the long-range dipole components of the force constants.

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