[QMS2020 invited talk]

Orbital-selective Mott and Peierls transition in hydrogenated VO_2

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Identifying low energy degrees of freedom and their interplay in correlated electron materials is a key to the understanding of their physical properties. For the metal-to-insulator-transitions (MIT) in particular, the strong electronic correlation plays a crucial role in the charge localization of the systems by an intricate interrelationship of lattice, charge, orbital, and spin degrees of freedom. In this talk, the mechanism of the recently reported MIT in hydrogenated H_xVO_2 will be discusssed, showing insulator to metal transition as increasing H doping and reentrance to the insulating phase in the fully hydrogenated limit (x=1). We investigate the electronic and optical properties of hydrogenated vanadium dioxide H_xVO_2. A hydrogenation-driven MIT is observed in the optical conductivity measured by spectroscopic ellipsometry, showing an optical gap opening at the Fermi level. The MIT is accompanied by a structural transition forming V-V dimers when complete hydrogenation is reached. The insulating phase of fully hydrogenated HVO_2 is investigated using density functional plus dynamical mean-field theory (DFT+DMFT). We identify the paramagnetic insulating phase in which both the Mott-gap opening with orbital ordering and the dimer-induced bonding-antibonding splitting is stabilized by on-site electronic correlations. We show that this simultaneous orbital-selective Mott and Peierls transition plays an important role in the MIT of H_xVO_2. The orbital structure of the insulating phase predicted by DFT+DMFT is further investigated by polarization-dependent optical conductivity and x-ray absorption measurements. Both measurements confirm the theoretically predicted orbital structures, providing a strong support to the Mott and Peierls insulating phase of HVO_2.