Pressure induced phase transition in correlated oxides and simple metals: Mott and charge-transfer insulators

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Pressure induced phase transition in correlated oxides and simple metals: Mott and charge-transfer insulators

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High pressure can radically change the behavior of simple substances. Consider sodium. At ambient pressures it has a symmetric crystal structure. Under large enough pressure, it changes from a shiny metal to a transparent insulator with several low-symmetry crystal structures. At very high pressures, the core electrons overlap and, because of the Pauli exclusion principle, give rise to less symmetric charge distributions. Coulomb repulsion between core and valence electrons localize charge in interstitial positions instead of at the nuclei, eventually leading to an insulating state. In this talk we will review the recent advances within density-functional and many-body based schemes to describe spectroscopic properties of complex systems with special emphasis to modeling the pressure (or light) induced phase transitions in correlated oxides and simple metals. Our first-principles calculations show that at pressures above the metal-insulator transition, sodium should be transparent in one polarization direction but reflective, like a normal metal, in the other. Photoluminescence experiments along the two axes of polarization should elucidate the nature of the bound exciton as well as the crystal structure at high pressures. We extended those studies to adder the pressure induce Mott insulator transition in MnO and well as the insulator-to-metal phase transition of VO_2. For the later we show that the band gap in monoclinic phase is extremely sensitive to small changes in the occupation of the localized d bands of V atoms. In particular, the photo-induced hole doping in VO_2 can strongly alter the dynamical screening, which then leads to a collapse of the band gap. Our results support the experimental findings and point to the electronic origin of the insulator-to-metal phase transition of monoclinic VO_2 in the time resolve photoelectron experiments.

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