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The electronic structure of the Mott insulator VO_2: the strongly correlated metal state is screened by impurity band. HYUN-TAK KIM, MIT Center in ETRI — A Mott insulator VO_2 ($3d^1$) has a direct gap ($\Delta_{direct} \propto V_{direct}$) of 0.6 eV and an indirect gap of $\Delta_{act} \propto V_{direct} \approx 0.15\ eV$ coming from impurity indirect band. At T_c, $\Delta_{direct} = \Delta_{act} = \mathrm{O}$ is satisfied and the insulator-to-metal transition (IMT) occurs. The metallic carriers near core region can be trapped when a critical onsite Coulomb U_c exists. Then, a potential energy is defined as

$$V_g = (V_{direct} + U_c) + V_{indirect}$$

$$= -(2/3)E_F(1 + e(N_{tot}/n_{tot})(1 - \exp(-\Delta_{\rm act}/k_B T))) + U_c, \quad (1)$$

where $V_{direct} = -(2/3)E_F$ is the screened Coulomb pseudopotential at K = 0. $\Delta\rho = \mathrm{N_{tot}/n_{tot}} \approx 0.018\%$ [1] is defined as the critical doping quantity, where n_{tot} is the carrier density in the direct band and N_{tot} is the carrier density in the impurity band. In $U_c < (2/3)E_F$ case, it sustains the insulator state. However, when both $U_c > (2/3)E_F$ and Δ_{act}= 0 by excitation are satisfied, the IMT occurs in $V_g \geq 0$. This indicates that the excitation ($\Delta_{act} = 0$) breaks the Coulomb equilibrium (V_g<0 and insulator sustaining U_c) in *Eq.* (1); the Coulomb energy changes from U_c to a $U < U_c$. The IMT can be switched by the doping (excitation; Δ_{act}= 0) and the de-doping (de-excitation; Δ_{act} =0.15 eV) of $\Delta\rho = \mathrm{N_{tot}/n_{tot}}$ to the conduction band, by applying external parameters such as heat, pressure, doping *etc.* The direct band gap (semiconductor gap) in the Mott insulator smaller than that of dielectric insulators can be explained by U_c.[1] NewJ.Phys.6(2004)52.

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