2016 / 11 / 15 (화) (1)

Orbital-selective effects in transition metal compounds

"molecules" in solids against magnetism.

Khomskii

- Peierls transition

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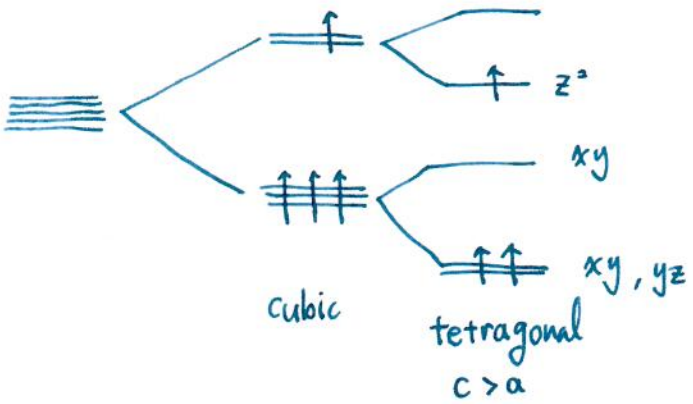
- strongly correlated electrons.

mott insulator.

$$H_{eff} = \frac{2t^2}{U} \sum_{\langle i,j \rangle} S_i \cdot S_j \qquad U/t \gg 1.$$



Physical scripta 72

crystal field splitting.

Jahn-Teller effect.

Goodenough - Kanamori - Anderson rule

1. Exchange interaction of two half-filled orbitals

Is strong and antiferromagnetic (AFM)

$$J_{AFM} = \frac{2t^2}{U}$$

2. Exchange interaction of half-filled and empty (or doubly-filled) orbitals is weak and ferromagnetic (FM)

$$J_{FM} = -\frac{2t^2 J_H}{U(U - J_H)}$$

"General rule" for 180° M - O - M angle.

Ferro orbitals $\Leftrightarrow$ antiferro spins

antiferro orbitals $\Leftrightarrow$ ferro spins

Has become a "common knowledge"
but be careful, only for 180°

For edge-sharing octahedra, 90° M - O - M angle,
the situation is very different!

3d pyro Nature materials 5, 471 (2006)

Spin gap in $NaTiSi_2O_6$ → PRL 96, 249701 (2006).