Mott transition

Synonym: Mott–Hubbard transition

A transition occurring only in 'single-valent' systems from strongly correlated ($U > W$) to weakly correlated ($U < W$) electrons as a result of a change of bandwidth W. W reflects the strength of the interatomic interactions in a periodic array of like atoms and U is a measure of the intra-atomic interactions, i.e. the electrostatic energy involved in the creation of polar states by transferring an electron from one atom to the next, as shown schematically by the disproportionation reaction:

$$M^{n+} + M^{n+} \rightarrow M^{(n+1)+} + M^{(n-1)+}$$

A $U > W$ produces a magnetic semiconductor; a $U < W$ gives rise to a metal (normally nonmagnetic). Note also that U and W can be altered by changes in interatomic distances, brought about through temperature or pressure variations or by introducing an alloying element. Synonymous with Mott–Hubbard transition.

Source:
PAC, 1994, *66*, 577 *(Definitions of terms relating to phase transitions of the solid state (IUPAC Recommendations 1994))* on page 587