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