Charge self-regulation upon changing the oxidation state of transition metals in insulators

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$$Q(q) = \sum_i \int_0^R r\, \psi_i^2$$

$$Q_B(q) = \sum_i^B \int_0^R r\, \psi_i^2$$

E[illegible] 4 [illegible] Q [illegible] Q_B [illegible] q. I[illegible] (E[illegible] 1) [illegible] Q [illegible] M [illegible] 0.2e [illegible] 1e [illegible] q. I[illegible] Q [illegible] M [illegible] Q [illegible] H[illegible] Q_B [illegible] M, [illegible] (E[illegible] 1), [illegible] Q [illegible] Q [illegible] M [illegible] C [illegible] 3d M [illegible] GaAs, C[illegible]$_2$O [illegible] MgO, [illegible] M- [illegible] 0.1e [illegible]

[illegible] Q_B [illegible] Q [illegible] E[illegible] 1 [illegible] M(γ) [illegible] M [illegible] M(γ) [illegible] E[illegible] 5 [illegible] ρ [illegible]

[illegible] M [illegible] GaAs ($\Delta\rho = \rho(0) - \rho(-1)$; E[illegible] 5 [illegible]), [illegible] +1 [illegible] C [illegible] C[illegible]$_2$O [illegible] MgO ($\Delta\rho = \rho(+1) - \rho(0)$; E[illegible] 5 [illegible]). I[illegible] M [illegible] (a [illegible] e) GaAs:M[illegible], C[illegible]$_2$O:C[illegible] [illegible] MgO:C[illegible] [illegible]), [illegible] Q [illegible] Q_B [illegible] E[illegible] 4 [illegible] E[illegible] 1.