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

Hannes Raebigerlators

[illegible] DB(γ) [illegible] (Eq. 1, [illegible]). [illegible] DB(γ) [illegible], [illegible] (Eq. 1, [illegible]). [illegible] M(γ) [illegible] DB(γ) [illegible], [illegible] (CFR) [illegible] M [illegible] (DBH) [illegible] p [illegible] M(γ) [illegible] DB(γ) [illegible], [illegible] Eq. 1, [illegible] Eq. 1 [illegible] Eq. 1

delithiated, the original TM^{3+} [illegible] $_2$ is M^{4+}. A [illegible] (C [illegible]). [illegible] F [illegible] (1) [illegible] ^{3} [illegible] RMO_3 [illegible] (R [illegible] L, [illegible] D) [illegible] C [illegible] M^{4+} [illegible] M^{3+} [illegible]; (2) [illegible] M [illegible] ^{3,4}; [illegible] (3) [illegible] M [illegible] ^{5} ([illegible]) M [illegible] M [illegible].

[illegible] M [illegible] MO [illegible] GAs, [illegible] 4/ (s)-5/ (/)-32 6(s)-33 12.275 s(/)11124 [illegible] s, s s-/. s / (-/)-3 .2(3 3(124 3(C E B 6.9488 0 0 6.1761 192.9(MO81256

[7,8,17] (Eq. 1). H [illegible] M(d) [illegible] n [illegible] γ ([illegible]) [illegible] $\gamma =$ ([illegible]) [illegible] $\gamma = e$ ([illegible])). [illegible] M(γ) (Eq. 1, [illegible]) [illegible]

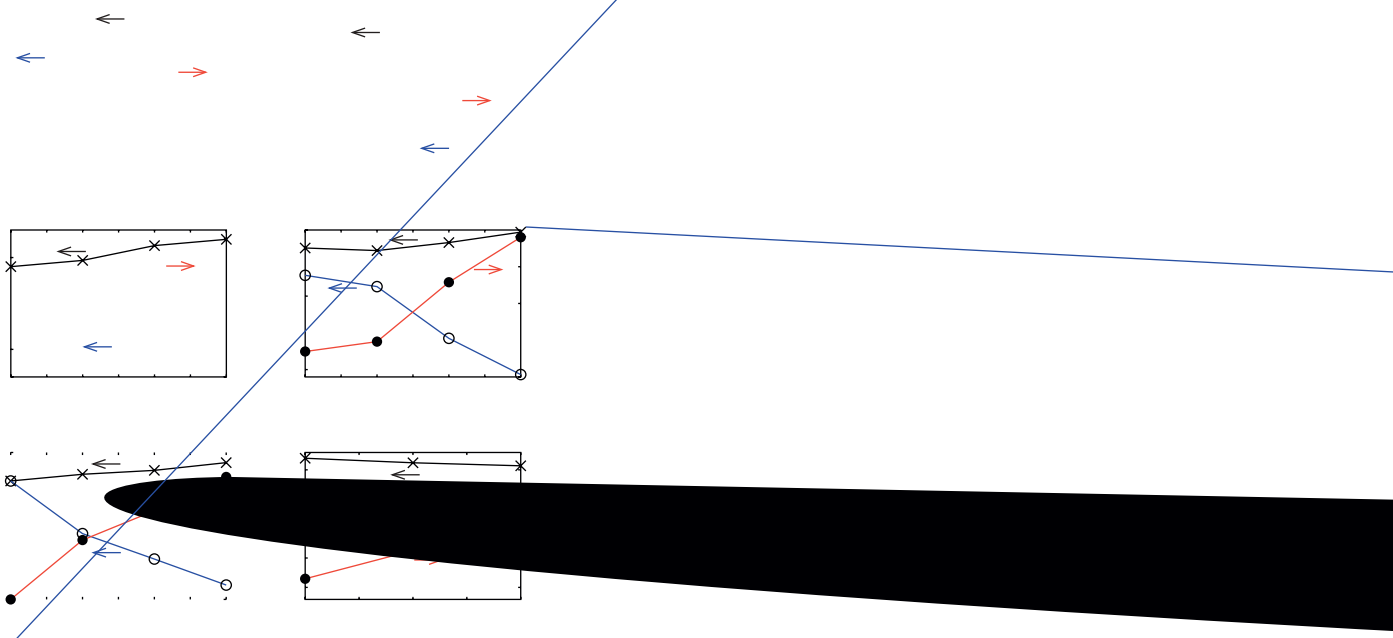
[illegible] CFR [illegible] M&t [illegible], [illegible] t DBH [illegible] M&t, [illegible]

$$Q_{\mathrm{A}}(q) = \sum_{i}^{\mathrm{A}} \int_0^R r\,\psi_i^2$$

$$Q_{\mathrm{B}}(q) = \sum_{i}^{\mathrm{B}} \int_0^R r\,\psi_i^2$$

E[illegible] 4s [illegible] Q_{tp}, Q_{A} [illegible] Q_{B} s [illegible] q. I [illegible] (E[illegible]. 1) [illegible] Q_{A} [illegible] M[illegible] 0.2e 1e [illegible] q. I [illegible] Q_{tp} [illegible] M[illegible] Q_{A} [illegible] H[illegible], [illegible] Q_{B} [illegible] M, [illegible] (E[illegible]. 1), [illegible] Q_{A} [illegible] Q_{tp} [illegible] M [illegible] 3d M[illegible] G[illegible]As, C_2O [illegible] M[illegible]O, [illegible] M- [illegible] 0.1e [illegible]

[illegible] Q_{B} [illegible] Q_{A} [illegible] E[illegible]. 1, [illegible] M(γ) [illegible] M[illegible] M(γ) [illegible] M[illegible] [illegible] E[illegible]. 5 [illegible] ρ [illegible] M[illegible] G[illegible]As ($\Delta\rho = \rho(0) - \rho(-1)$; E[illegible]. 5), [illegible] -+1 [illegible] C[illegible] C_2O [illegible] G[illegible] M[illegible]O ($\Delta\rho = \rho(+1) - \rho(0)$; E[illegible]. 5 ,). I [illegible] M[illegible] [illegible] G[illegible]As:M[illegible], C_2O:C[illegible] M[illegible]O:C[illegible], [illegible] Q_{A} [illegible] Q_{B}s, [illegible] E[illegible]. 4 [illegible] E[illegible]. 1.



E [illegible] t [illegible] M, [illegible] A [illegible] M [illegible] CFR [illegible] (E [illegible] 1),