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ad a c d ΔH_D. S c d, ca c a d d c, ΔH_D,
d d a F (a (1

. . E_F = $_{VBM}$ + ΔE_F, ΔE_F d F
c d c ba d a (0 < ΔE_F < E).
S c (d) a a c a c ( ) a c
c a ac a [56

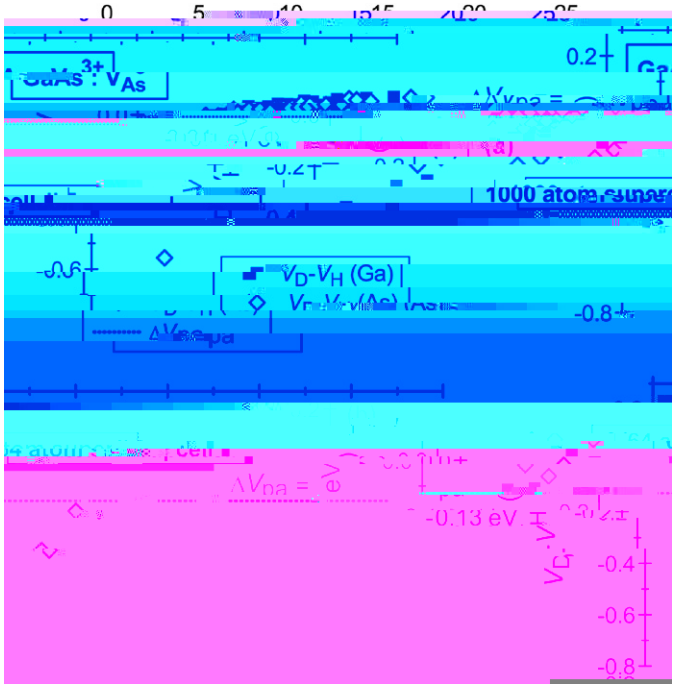

Figure 1. T d c a c , a , V_{Ga} a d V_A b a, t c c a a aca c V_A^{3+} a d d c - , 1000 a t c (*a*) a d a 64 a t c (*b*).

Add , , a ca c t , ac tt ($\varepsilon = 1$), Ma- a d Pa d d a , , a d d c c b d c , a c a a , c a t a d d ( ), t a d , ($\boldsymbol{r}$). I , ca , c c d t ($\boldsymbol{r}$) a , -c a a , (ad t ac),

$$\Delta E_{\text{}}^{3} = \frac{2 \quad Q}{3\varepsilon L^{3}}, \tag{6}$$

$$Q = \int \mathrm{d}^{3} \quad (\boldsymbol{r})^{2} \tag{7}$$

, , c d ad a d d c a d , . S c , ca c t , ac , ($\boldsymbol{r}$), c a d , c , b ($\boldsymbol{r}$) a d , a , (t , -c a c b t), ca , a $O(L^{-5}$

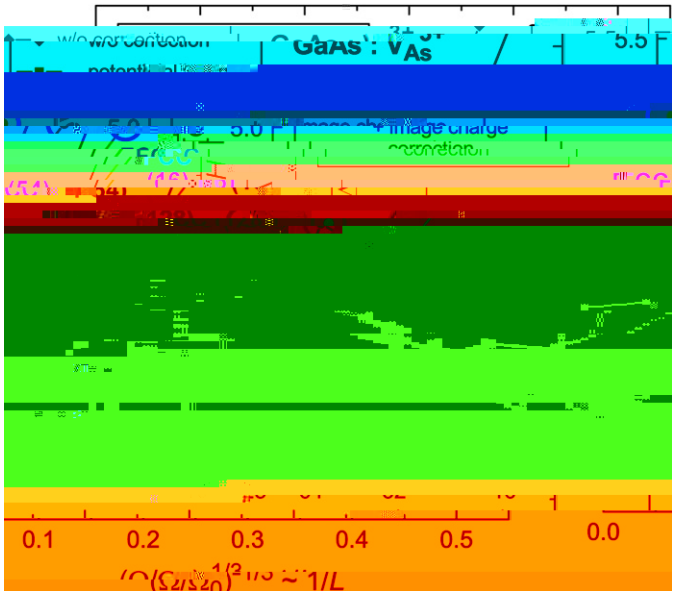

Figure 2. T a ΔH V_A^{3+} d c GaA ($E_F = E_V$, A -c c d) a a t c a t c d 1/L = $^{-1/3}$ (= t c t , $_0$ = t 2 a GaA t c). (M d d [25].)

a c a d a c d z - c a [25]. L a c c a b d ac -c d c bc (FCC) t c (. ., 16, 54, 128 a), c a a b d ac a t d c a a d a (1 1 0) - a c a , c d c d c. d c ac . C t , t c a c d d d c ca c a .

W a c a c c acc d a (5) (7) d t cc t , a c c a ca c d c , c add . F , a Q (a (7)), t d c a a a Δ D(r) a d a c c . H , t d [25] a Q

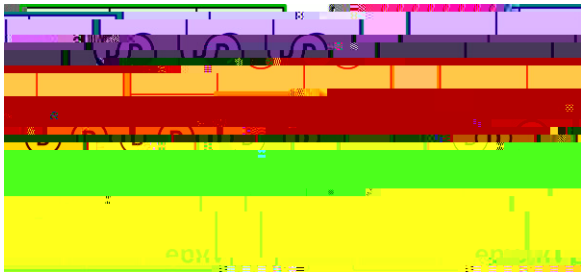

Figure 3. Sc a c t a a d c t c ( ) a ( ) , dc a ( ) a c ( ).

d ca d c t c (z t 3):

$$\Delta E = -\int \mathrm{d}^3(\rho_H(\boldsymbol{r}) + \Delta\rho(\boldsymbol{r}) + \Delta\rho_D(\boldsymbol{r}))\int \mathrm{d}^3\frac{\Delta\rho(\boldsymbol{r}') + \Delta\rho_D(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}. \tag{8}$$

U d a a a c , a t a ac t c t a a, a t a b c ca c (d b d a d a c), ca c ac $\rho_H(\boldsymbol{r})$ a d c d c dd t [$\Delta\rho(\boldsymbol{r}') + \Delta\rho_D(\boldsymbol{r}')$] a c . T , c d $\rho_H(\boldsymbol{r})$, ca a (8) a ac b a d D:

ΔE

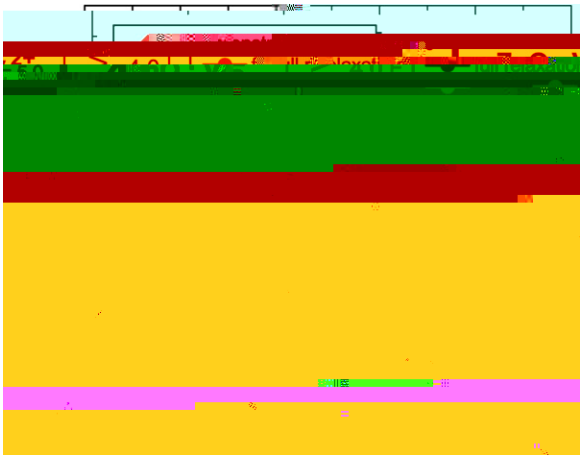

Figure 4. F , ca ΔH V_O^{2+} d c Z O (E_F = E_V, O- c) GGA, ca c a d c , a d a c a a (d a d) a d t a a (o ç ,). T a c a c c , d d t , ε_∞ = 5.0 ε_0 = 10.3.

a, c b t , , c a c a , a a (c c+ c), . . - c d c c c , a $\varepsilon = \varepsilon_0$, a , a , , d a t c d , , t o a c a d c , c . U , 72, 192 a d 576 a , c , t a c , , 4 , ca V_O^{2+} Z O, , a a d c b ε_0 a d ε a , . ., GaA . W d ε = 5.0 a ca c a a , d ca

c c , d c a b -c , LDA d c ca c a [6, 18, 22, 25]. I a ca , , a ba d a ad a , t t b d a b d c , a , a d , ba d , ad a a , a , d , c , d c , a [27]. I , ca , , a c c , -c , ca c a , d , ab . I d c c ba d , c , c d c , -c , ca c a , C , [51], d c d add a a , c , ca ad d a c a ba d , c . I a , a , ,

A d c b NLEP a d LDA+*U*, a a- c b d NLEP a , d d a d c c ac . W a LDA + *U*, d d a (c d) Ha . F c- ac [61, 62], NLEP a a d a , a . S c , ac b c , a d a a , c a d cc d a , add a ,