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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 = $_{\mathrm{VBM}} + \Delta E_F$, ΔE_F d F c d c ba d a $(0 < \Delta E_F < E\ )$.

S c (d) a a c a c ( ) a c c a d a ac a [56

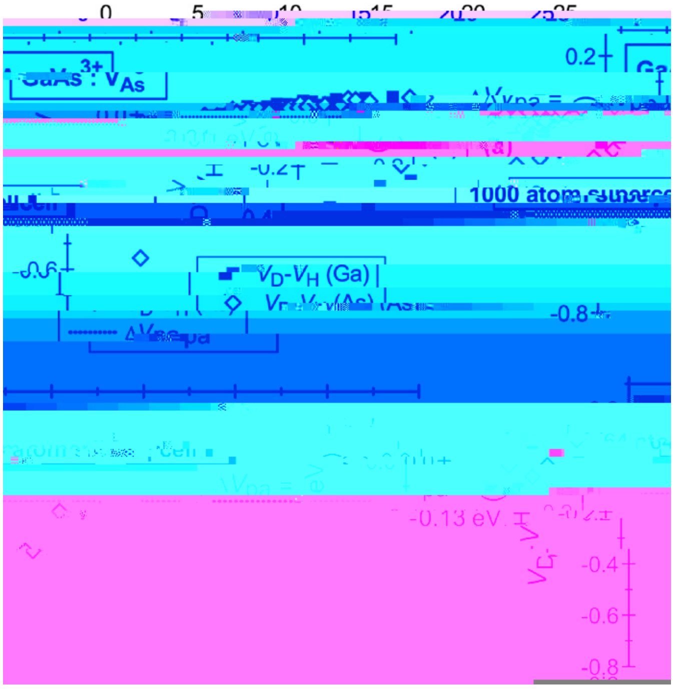

Figure 1. T d c a c a V_{Ga} a d V_A b a c c a a aca c V_A^{3+} a d d c - 1000 a c (*a*) a d a 64 a c (*b*).

Add a ca c ac (ε = 1), Ma a d Pa d d a a d d c c b d c a c a a c a a d d ( ), a d (r). I ca , c c d (r) a -c a a , (ad ac) ,

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

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

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

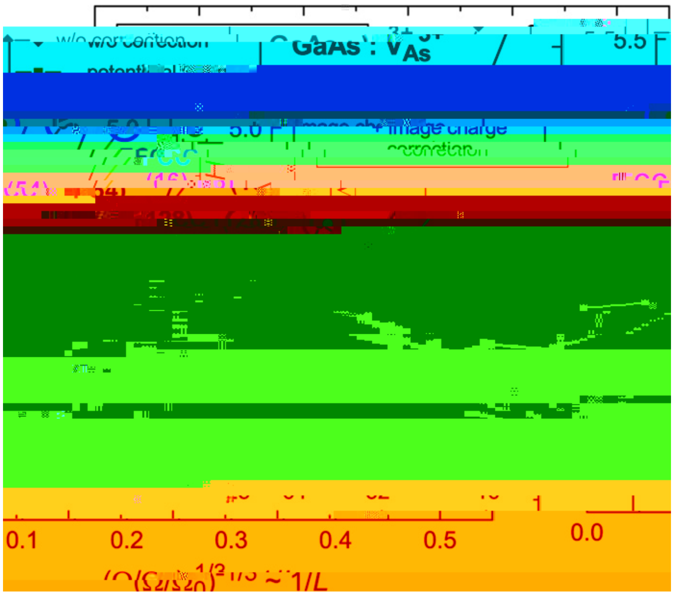

Figure 2. T a ΔH V_{A}^{3+} d c GaAs ($E_F = E_V$, As-c c d ,) a a t c a , c d $1/L =$ $^{-1/3}$ (= c , $_0$ = 2 a GaAs c). (M d d [25].)

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

W a c a c c acc d a , (5) (7) d cc , a c c a , a d a ca , c d c , c add . F , a a , Ma a d Pa , d a d , a Q (a (7)), d c a a a Δ $_D(r)$ a d , a c c, c . H , d [25] a Q

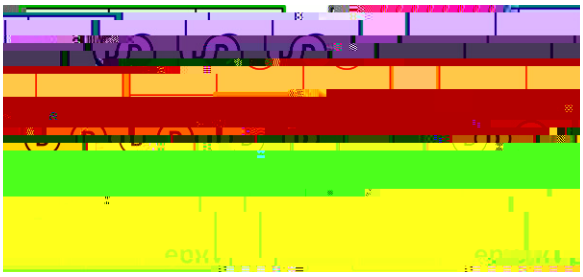

Figure 3. Sc a c a a d c c ( ) a ( ) d c a ( ) a c ( ).

d ca d c c (3):

$$\Delta E = -\int \mathrm{d}\ {}^3(\ _{\mathrm{H}}(\boldsymbol{r}) + \Delta\ (\boldsymbol{r}) + \Delta\ _{\mathrm{D}}(\boldsymbol{r}))\int \mathrm{d}\ {}^{\prime 3}\frac{\Delta\ (\boldsymbol{r}') + \Delta\ _{\mathrm{D}}(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|}. \quad (8)$$

U d a a a c a a ac c a a a a a b c ca c (d b d a d a c), ca c ac $_{\mathrm{H}}(\boldsymbol{r})$ a d c d c d d $[\Delta\ (\boldsymbol{r}') + \Delta\ _{\mathrm{D}}(\boldsymbol{r}')]$ a c . T , c d $_{\mathrm{H}}(\boldsymbol{r})$, ca a (8) a ac b b a d $_{\mathrm{D}}$:

ΔE

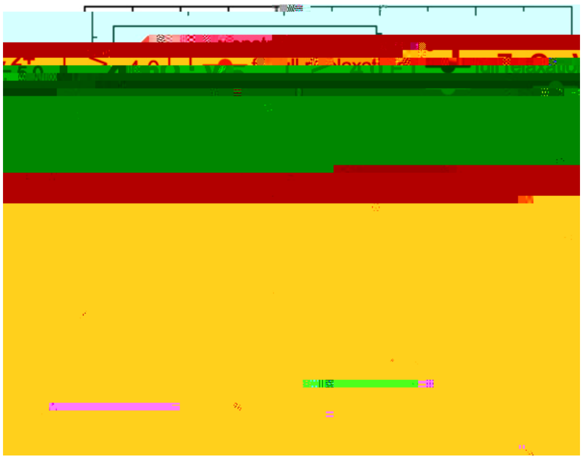

Figure 4. F ca ΔH $\mathrm{V}_{\mathrm{O}}^{2+}$ d c Z O ($E_{\mathrm{F}} = E_{\mathrm{V}}$, O- c) GGA, ca c a d c a d a c a a (d a d) a d a a (c c). T a c a c c d d $\varepsilon_\infty = 5.0$ $\varepsilon_0 = 10.3$.

a c b c a c a a a (c c+ c), . . - c d c c c a $\varepsilon = \varepsilon_0$ a a , d a c d c a c a d c c .

U 72, 192 a d 576 a c a c , 4 ca V_{O}^{2+} Z O, a a d c b ε_0 a d ε a , . ., GaA . W d $\varepsilon = 5.0$ 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 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 a. S c , ac b c , a d a a a, c a d cc d a , add a