

## Accurate prediction of defect properties in density functional supercell calculations

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ad a c d ,  $\Delta H_D$ . S c d , c a d d c ,  $\Delta H_D$ ,  
d d a F a (1

$E_F = E_{VBM} + \Delta E_F$ ,  $\Delta E_F$  d  $F$   $(0 < \Delta E_F < E)$ .  
 S c t ( d ) a a c ( ) a c [56]



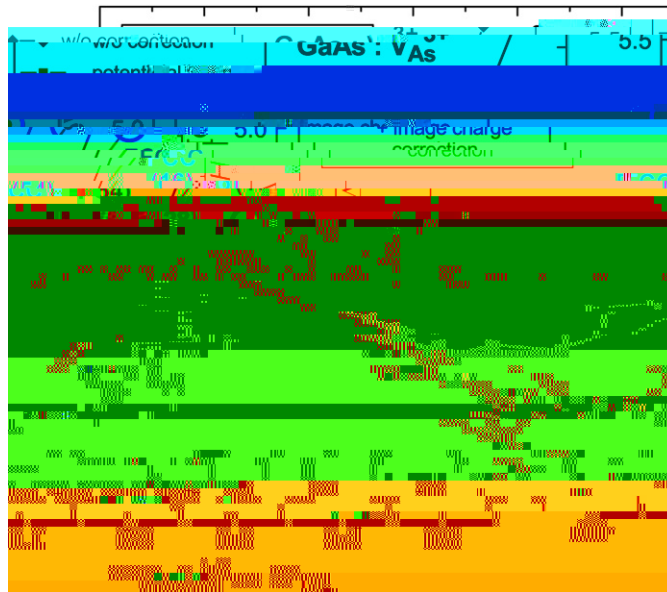


Figure 2. T a s ΔH V<sub>A</sub><sup>3+</sup> d c s GaAs (E<sub>F</sub> = E<sub>V</sub>, A<sub>s</sub> - c c d s , ) a  
 a t c s , / j s a t c s j d s 1/L = <sup>-1/3</sup> ( = t c s j t , 0 =  
 j t 2 a GaAs t c s j ). (M d z d [25].)

a c , a d , a c t d z , z , c , s a j a c s , [25].  
 L , a s c c a b d j ac -c d c b c (FCC), t c s  
 ( . . , 16, 54, 128 a s ), c a a b d ac a s , s ,  
 d c , a a d a (110) , - a c a t , c . d c d c .  
 d c , ac . C t j , / t c s a a j c d d d c  
 c a c a s .  
 W j , a c a c c s acc d a s , (5) (7) d t cc t j ,  
 j a c c s a t a d a a c a s , c d c s c t j ,  
 add . F , s s a a , Ma a d Pa t j d a t d s ,  
 s a Q ( t a s (7)), t j d c a j a a Δ<sub>D</sub>(r) a d ,  
 a s j c s c s . H , t d s [25] a Q







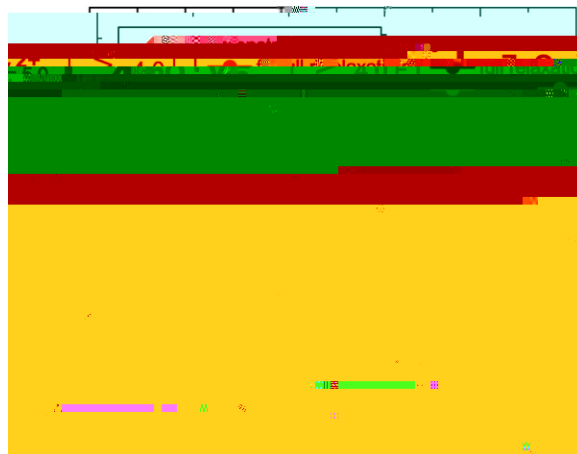


Figure 4.  $\Delta H$   $V_O^{2+}$  d c , Z O ( $E_F = E_V$ , O-c), GGA,  $\epsilon = 5.0$   $\epsilon_0 = 10.3$ .

a, c b t , c , a c a a a ( c c+ c),  
 . . . t c d c c c a  $\epsilon = \epsilon_0$  a , a , d a c  
 d t a c a d , c , c .  
 U, 72, 192 a d 576 a t c  
 t a a d c b  $\epsilon_0$  a d  $\epsilon$   
 a , . . , GaAs. W d ,  $\epsilon = 5.0$  a c a , a , d c a,

c c , d c a b t -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 . I d c c ba d c c d c  
ca c a , C [51] d c d add a a , c  
ca ad d a c a ba d t c . I a a ,

A d c b NLEPa dLDA+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, t, cc, d, a, add, a,





