

Accurate prediction of defect properties in density functional supercell calculations

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

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

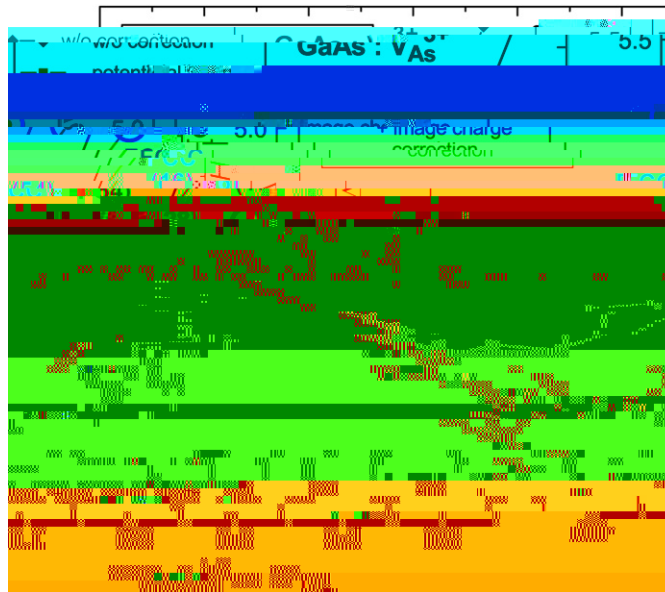


Figure 2. T a s ΔH V_A³⁺ d c s GaAs (E_F = E_V, A_s - c c d s ,) a
 a t c s , / j s a t c j j d s 1/L = ^{-1/3} (= t c j j t , 0 =
 j t 2 a GaA t c j j). (M d z d [25].)

a c , a d , a c t d z , z , c , s a j a c s , [25].
 L , a , c c a b d j ac -c d c b c (FCC), t c j j
 (. . , 16, 54, 128 a ,), c a a b d ac a , 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 j j a a j c d d d c
 c a c t a , .
 W j , a c a c c , acc d a s , (5) (7) d t c c t j ,
 j a c c , a t , a d a a , ca , s , c d c , c t j ,
 add . F , s , j a , a , Ma a d Pa t j d a t d ,
 , a Q (t a (7)), t j d c a j a a Δ_D(r) a d ,
 a , j c , c s . H , t d [25] a Q

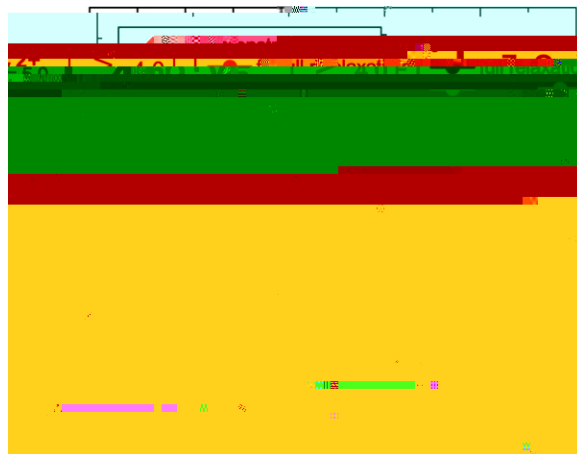


Figure 4. ΔH V_O^{2+} d c , Z O ($E_F = E_V$, O-c), GGA, $\epsilon = 5.0$ $\epsilon_0 = 10.3$.

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 ϵ_0 a d ϵ
 a , . . , GaAs. W d , $\epsilon = 5.0$ a c a , a , d c a,

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 . 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, c a d, t, cc, d, a, add, a,

