



removal energies  $\varepsilon_{\text{ok}}(q \rightarrow q+1)$  higher

1(2),  $V_{\text{ok}}^0(a_1^2) \rightarrow V_{\text{ok}}^{1+}(a_1^1) \rightarrow V_{\text{ok}}^{2+}(a_1^0)$ ; addition

energies  $\varepsilon_{\text{ok}}(q \rightarrow q-1)$  lower

$V_{\text{ok}}^{2+}(a_1^0) \rightarrow V_{\text{ok}}^{1+}(a_1^1) \rightarrow V_{\text{ok}}^0(a_1^2)$ . B  $\varepsilon(q/q')$ . H  $V_{\text{ok}}^{2+}$  [F 1(1)],

(A)  $\text{DF}$  16

17) GW<sup>18</sup> 2 19. F (B)

20 ( ) 21 F

DF GW GGA

22  $\text{DF} + U$  23  $\text{GGA} + U$

$J=6$   $\text{GW} - \text{GGA} + U$

$\text{GGA} + U$  F 1,

$V_{\text{ok}}^I$  GGA (  $U$  )  $V_{\text{ok}}$

2

$\text{GW}$   $\text{GGA}$

24 F H E -DF

25 (  $\text{GW} - \text{H E}$  ),  $\alpha=0.25$

F  $\mu=0.2$

F (A)  $\text{DF}$

$R=1.0$  )  $\text{DF}$

( 2 ) -DF ( 8 ) [

( 2 ) ( 8 ) ] B

$$e_n^{GW} = e_n^{DF} - \langle \psi_n^{DF} | \Sigma(e_n^{GW}) - V^{DF} | \psi_n^{DF} \rangle, \quad (1)$$

DF  $\psi_n^{DF}$  ( $n=1, 2, \dots$ )  
 GW  $\Sigma$   
 W ( $\epsilon_1$ )  
 GW (GW-H E), 3.25 (GW-GGA+U)  
 3.34 (GW-H E),  
 14,26  $F_{ii} = 1$   
 $a_1$   $V_{\text{xc}}$   
 $a_1$   $V_{\text{xc}}$   
 $a_1$   $B(E)$   
 CB ( $E_C$ )  
 CB  $B$   
 4  $I$   
 [S. Fil. 1( )].  
 1  
 B  $-d$   
 DF +U  $-d$   
 3,13  
 I  $V_{\text{xc}}^{2+}$   $a_1$

$\epsilon(\alpha=0.25)$  CB

Absolute formation energies.  $B_{\text{site}}$   $V_{\text{site}}$   $GGA+U$   $H$   $E$   $V_{\text{site}}^0$   $\epsilon(q/q')$   $\Delta H(V_{\text{site}}^q)$   $F$   $3$   $GGA+U$   $U$   $28$   $\Delta H(V_{\text{site}}^0)=0.81$   $GGA+U$   $H$   $E$   $\alpha$