

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

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

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

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

(A) DF^{16}

17) GW¹⁸ 2 19. F (B)

DF^{20} () DF^{21} F

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

U $J=6$ GGA+U

GW-GGA+U. GGA+U F. 1,

V_{ion}^I GGA (U) V_{ion}^I

$1+s$ DF^{24} GGA

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

F $\mu=0.2$

F (A) DF

$R=1.0$) DF^{26} (2) DF^{27} (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 ψ_n^{DF} ($n=1, 2, \dots$)
 GW Σ
 W (ϵ_1)
 GW (GW-H E), 3.25 (GW-GGA+U)
 3.34 F_{11} 1 a_1 V_{xc}
 a_1 V_{xc}
 a_1 $B(E)$ $B(E_C)$ B
 I 4 I B
 I $[S, F, 1()]$
 I 1
 B $-d$ $-p$
 I $DF + U$ $-d$
 I V_{xc}^{2+} a_1

$\epsilon(\alpha=0.25)$ CB

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