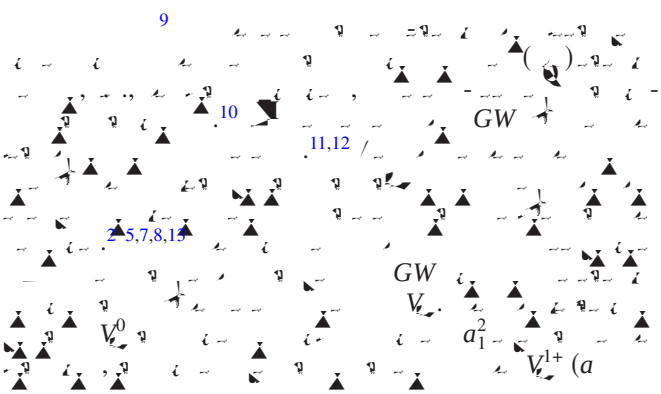

E . removal energies ε(q→q+1) higher [., $V_v^0(a_1^2)\to V_v^{1+}(a_1^1)\to V_v^{2+}(a_1^0)$; . 1( )] , . 12, addition energies ε(q→q. 1) lower [., $V_v^{2+}(a_1^0)\to V_v^{1+}(a_1^1)\to V_v^0(a_1^2)$]. ε(q/q′). , a_1 V^{2+} [. 1( )], . J ( ), J (A) A , [16] 17) GW.[18] - . 2 19. ( ) ,[20] ( ) .[21] , GW - E , A . [22] +U [23] -d - U J17(

$$e_n^{GW} = e_n + \langle \psi_n | \Sigma(e_n^{GW}) \cdot V | \psi_n \rangle, \qquad (1)$$

ψ_n ($n=$) GW Σ ( ) G W ( ). GW 3.25 (GW- A+U) 3.34 (GW-), GW .[14,26] 1 a_1 V V V .[5] a_1 (E) (E) GW .[4] [. 1( )]. J -.[1] -d -p +U -d .[3,13] V^{2+}, a_1 A+U GW, [3,13] V . [. 1( ) J s- . 3 A .]

GW-corrected thermodynamic transition energies. / ε GW E A+U ε(q/q′). :[19] $V^{1+} \rightarrow V^{2+} + e$ [. 1( )], V^{2+} 1+ 2+ 1+ (( ). - 1346 57.78 0 J/ 5 - 1 3 J/ -268.73.1098 - 46 5

(α=0.25) 1

Absolute formation energies.

V_z, [4,5,7,8,13]

GW

V_z^0

A+U

$\varepsilon(q/q')$

$\Delta H(V_z^q)$, . 3( ).

A+U,

U

. 28,

$\Delta H(V_z^0)$=0.81

A+U,

α (