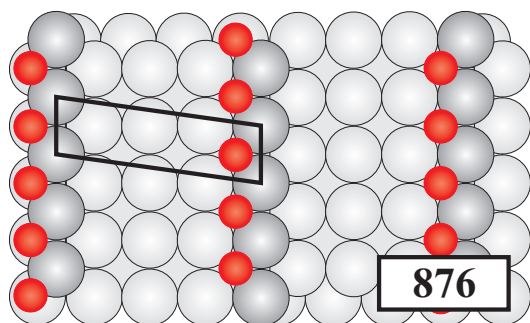


# Appendix F

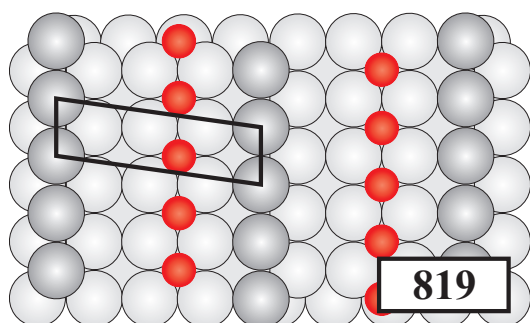
## Computed Ordered Configurations for O-Pd(117)

Listed are all ordered configurations of O at Pd(117) that were computed by (L)APW+lo DFT. Shown is a schematic top view indicating the surface unit-cell. The computed DFT total binding energy is given in meV, and the LGH expansion using all cluster figures in the considered pool (Fig. 8.1) is stated. Light grey spheres represent Pd atoms, while the Pd step atoms are shown in grey, to better illustrate the step structure in the top view, and dark (red) spheres represent O atoms.



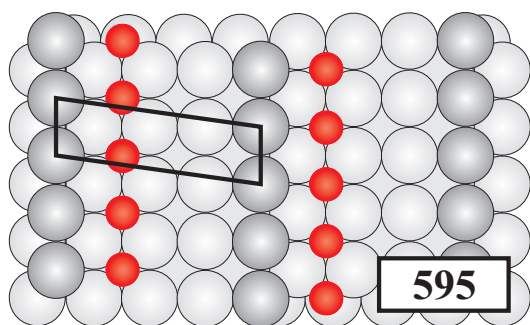
**V7-1**

$$E_b^{V7-1} = E_{b,Thu}^{On-site} + V_{1p}^{11} + V_{3p}^{11} + V_{1t}^{111}$$



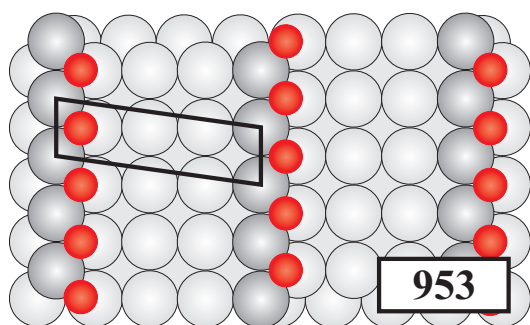
**V7-2**

$$E_b^{V7-2} = E_{b,The}^{On-site} + V_{1p}^{22} + V_{3p}^{22} + V_{1t}^{222}$$



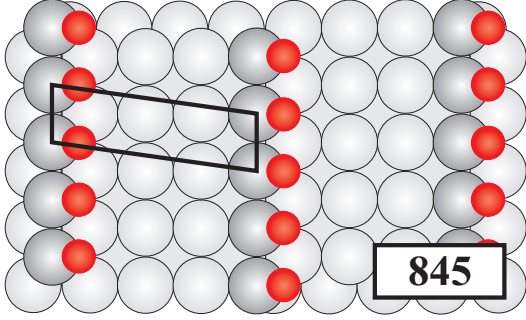
**V7-3**

$$E_b^{V7-3} = E_{b,Thl}^{On-site} + V_{1p}^{33} + V_{3p}^{33} + V_{1t}^{333}$$

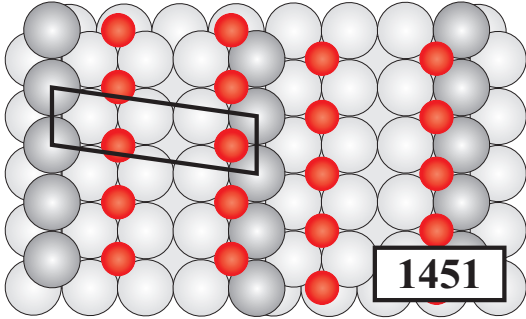


**V7-4**

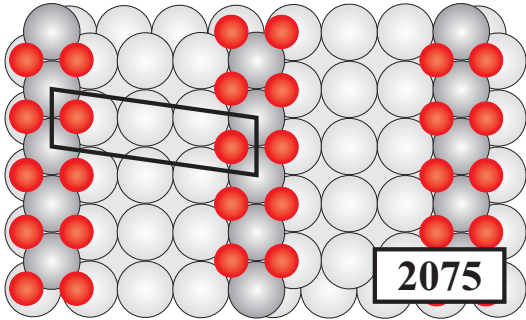
$$E_b^{V7-4} = E_{b,Sh2}^{On-site} + V_{1p}^{44} + V_{3p}^{44} + V_{1t}^{444}$$


**V7-5**

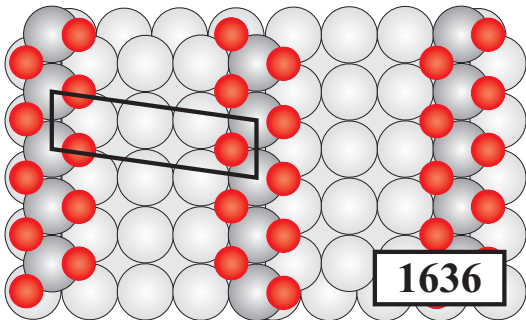
$$E_b^{V7-5} = E_{b,Sh1}^{On-site} + V_{1p}^{55} + V_{3p}^{55} + V_{1t}^{555}$$


**V7-6**

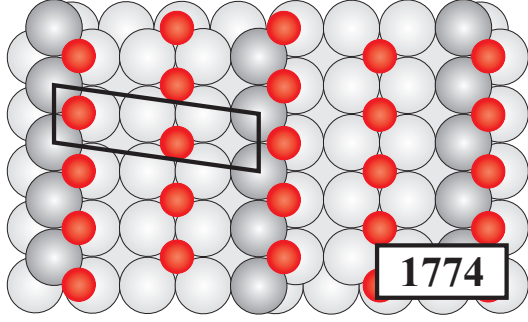
$$E_b^{V7-6} = E_{b,Thu}^{On-site} + E_{b,Thl}^{On-site} + V_{1p}^{11} + V_{3p}^{11} + V_{1p}^{33} + V_{3p}^{33} + V_{3p}^{13} + V_{3cp}^{13} + V_{1t}^{111} + V_{1t}^{333}$$


**V7-7**

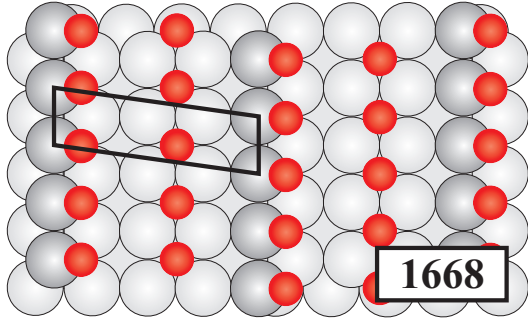
$$E_b^{V7-7} = E_{b,Thu}^{On-site} + E_{b,Sh2}^{On-site} + V_{1p}^{11} + V_{3p}^{11} + V_{1p}^{14} + 2V_{2p}^{14} + V_{1p}^{44} + V_{3p}^{44} + V_{1t}^{111} + 2V_{2t}^{114} + 2V_{2t}^{144} + V_{1t}^{444} + 2V_{3t}^{114} + 2V_{3t}^{144}$$


**V7-8**

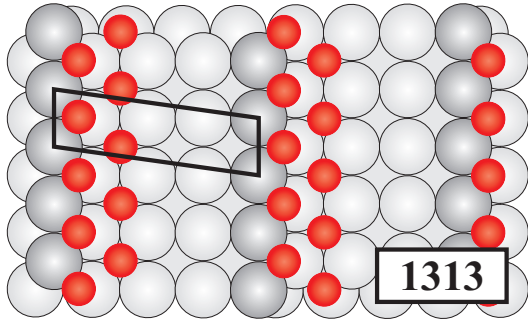
$$E_b^{V7-8} = E_{b,Thu}^{On-site} + E_{b,Sh1}^{On-site} + V_{1p}^{11} + V_{3p}^{11} + V_{1p}^{55} + V_{3p}^{55} + 2V_{2p}^{15} + 2V_{3p}^{15} + V_{1t}^{111} + 2V_{2t}^{115} + 2V_{2t}^{155} + 2V_{3t}^{115} + 2V_{3t}^{155} + V_{1t}^{555}$$


**V7-9**

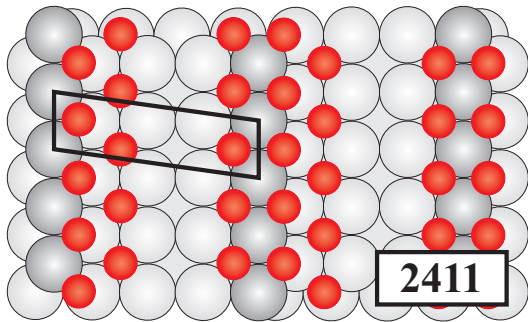
$$\begin{aligned}
 E_b^{V7-9} = & E_{b,Thc}^{On-site} + E_{b,Sh2}^{On-site} + V_{1p}^{22} + V_{3p}^{22} + V_{1p}^{44} \\
 & + V_{3p}^{44} + V_{3p}^{24} + 2V_{3p}^{24} \\
 & + V_{1t}^{222} + V_{1t}^{444}
 \end{aligned}$$


**V7-10**

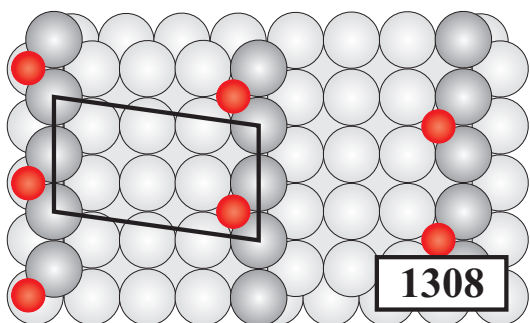
$$\begin{aligned}
 E_b^{V7-10} = & E_{b,Thc}^{On-site} + E_{b,Sh1}^{On-site} + V_{1p}^{22} + V_{3p}^{22} + V_{3p}^{25} \\
 & + V_{1p}^{55} + V_{3p}^{55} + V_{1t}^{222} + V_{1t}^{555}
 \end{aligned}$$


**V7-11**

$$\begin{aligned}
 E_b^{V7-7} = & E_{b,Thl}^{On-site} + E_{b,Sh2}^{On-site} + V_{1p}^{33} + V_{3p}^{33} + V_{1p}^{44} + V_{3p}^{44} \\
 & + 2V_{2p}^{34} + 2V_{3p}^{34} + V_{1t}^{333} + V_{1t}^{444} + V_{2t}^{334} + V_{2t}^{344} \\
 & + V_{3t}^{334} + V_{3t}^{344}
 \end{aligned}$$

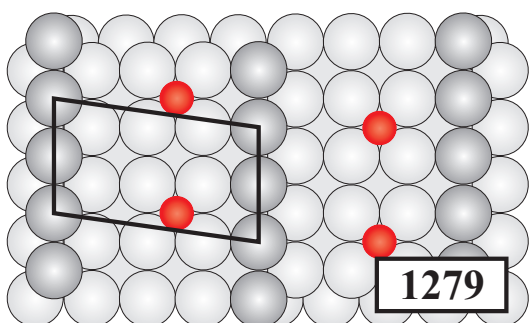

**V7-12**

$$\begin{aligned}
 E_b^{V7-12} = & E_{b,Thu}^{On-site} + E_{b,Thl}^{On-site} + E_{b,Sh2}^{On-site} + V_{1p}^{11} + V_{3p}^{11} \\
 & + V_{1p}^{14} + 2V_{2p}^{14} + V_{1p}^{33} + V_{3p}^{33} + V_{3p}^{13} + 2V_{3p}^{13} \\
 & + V_{1p}^{44} + V_{3p}^{44} + 2V_{2p}^{34} + 2V_{3p}^{34} + V_{1t}^{111} + V_{1t}^{333} \\
 & + V_{1t}^{444} + 2V_{2t}^{114} + 2V_{2t}^{144} + 2V_{2t}^{334} + 2V_{2t}^{344} \\
 & + 2V_{3t}^{114} + 2V_{3t}^{144} + 2V_{3t}^{334} + 2V_{3t}^{344} + 2V_{3t}^{134} \\
 & + 2V_{3t}^{134}
 \end{aligned}$$



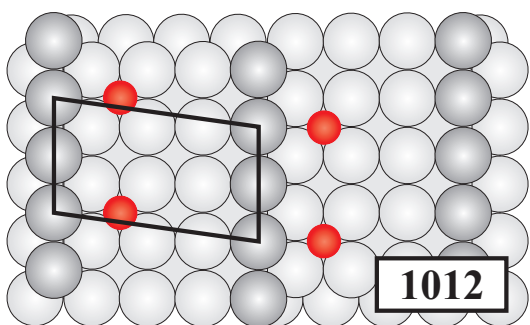
**V7-13**

$$E_b^{V7-13} = E_{b,Thu}^{On-site} + V_{3p}^{11}$$



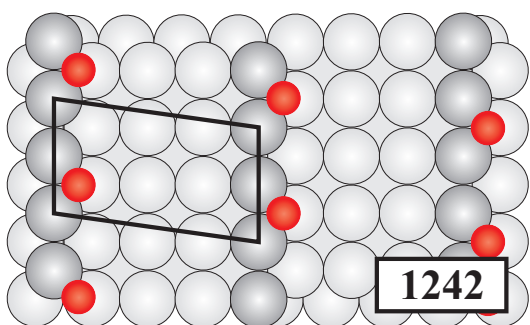
**V7-14**

$$E_b^{V7-14} = E_{b,Thc}^{On-site} + V_{3p}^{22}$$



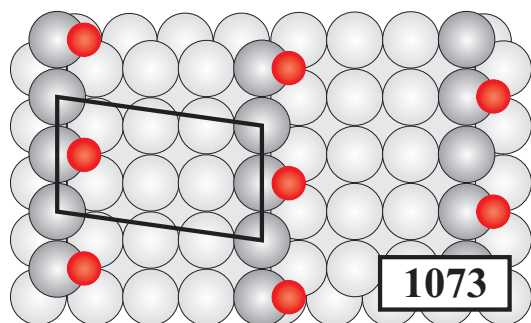
**V7-15**

$$E_b^{V7-15} = E_{b,Thl}^{On-site} + V_{3p}^{33}$$



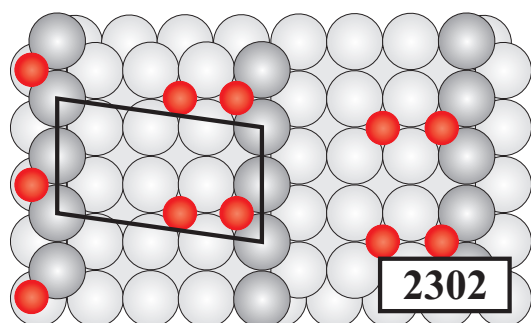
**V7-16**

$$E_b^{V7-16} = E_{b,Sh2}^{On-site} + V_{3p}^{44}$$



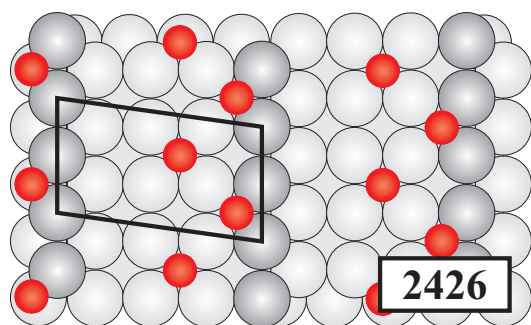
**V7-17**

$$E_b^{V7-17} = E_{b,sh1}^{\text{On-site}} + V_{3p}^{55}$$



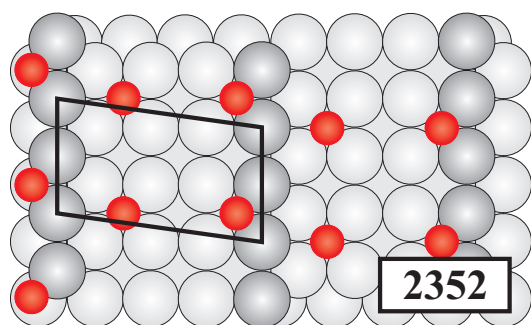
**V7-18**

$$E_b^{V7-18} = E_{b,Thu}^{\text{On-site}} + E_{b,Thc}^{\text{On-site}} + V_{3p}^{11} + V_{3p}^{22} + V_{1p}^{12}$$



**V7-19**

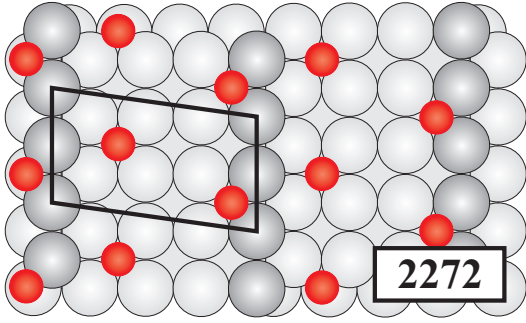
$$E_b^{V7-19} = E_{b,Thu}^{\text{On-site}} + E_{b,Thc}^{\text{On-site}} + V_{3p}^{11} + V_{3p}^{22} + 2V_{2p}^{12}$$



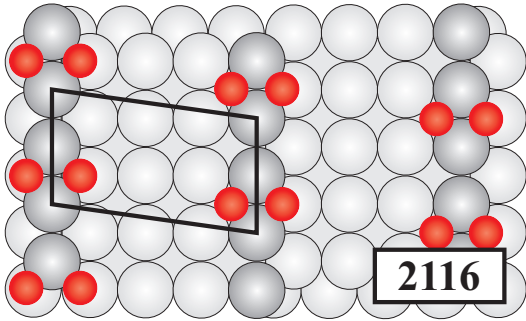
**V7-20**

$$E_b^{V7-20} = E_{b,Thu}^{\text{On-site}} + E_{b,Thl}^{\text{On-site}} + V_{3p}^{11} + V_{3p}^{33} + V_{3p}^{13} + V_{3cp}^{13}$$

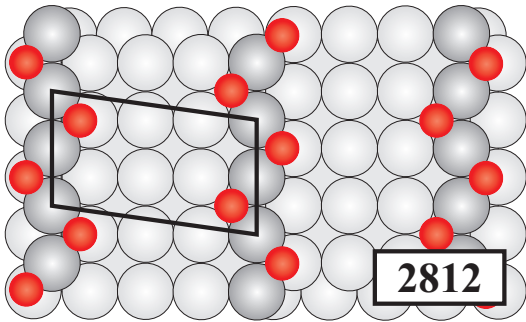



**V7-21**

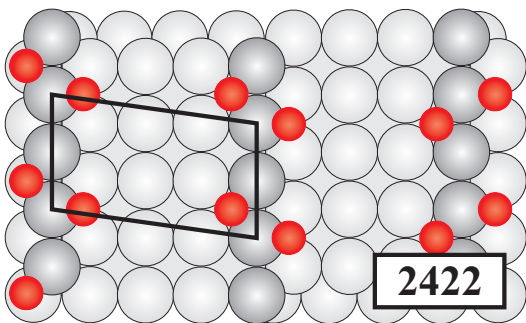
$$E_b^{V7-21} = E_{b,Thu}^{\text{On-site}} + E_{b,Thl}^{\text{On-site}} + V_{3p}^{11} + V_{3p}^{33} + V_{3cp}^{13}$$


**V7-22**

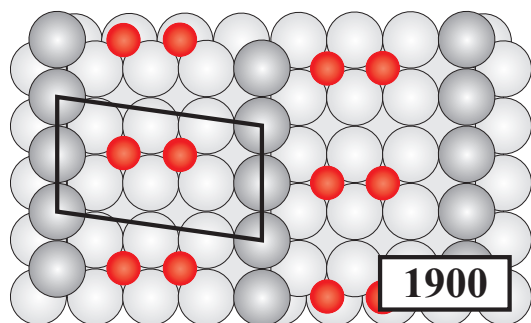
$$E_b^{V7-22} = E_{b,Thu}^{\text{On-site}} + E_{b,Sh2}^{\text{On-site}} + V_{3p}^{11} + V_{3p}^{44} + V_{1p}^{14}$$


**V7-23**

$$E_b^{V7-23} = E_{b,Thu}^{\text{On-site}} + E_{b,Sh2}^{\text{On-site}} + V_{3p}^{11} + V_{3p}^{44} + 2V_{2p}^{14}$$

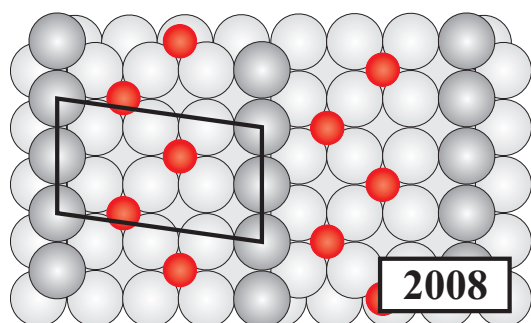

**V7-24**

$$E_b^{V7-24} = E_{b,Thu}^{\text{On-site}} + E_{b,Sh1}^{\text{On-site}} + V_{2p}^{15} + V_{3p}^{11} + V_{3p}^{15} + V_{3p}^{55}$$



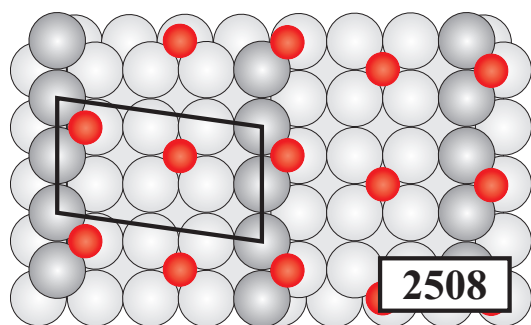
**V7-25**

$$E_b^{V7-25} = E_{b, \text{The}}^{\text{On-site}} + E_{b, \text{Thl}}^{\text{On-site}} + V_{1p}^{23} + V_{3p}^{22} + V_{3p}^{33}$$



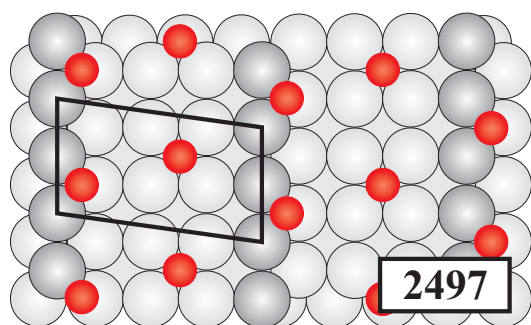
**V7-26**

$$E_b^{V7-26} = E_{b, \text{The}}^{\text{On-site}} + E_{b, \text{Thl}}^{\text{On-site}} + 2V_{2p}^{23} + V_{3p}^{22} + V_{3p}^{33}$$



**V7-27**

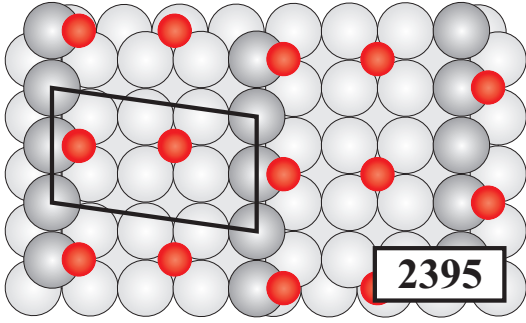
$$E_b^{V7-27} = E_{b, \text{The}}^{\text{On-site}} + E_{b, \text{Sh2}}^{\text{On-site}} + V_{3p}^{22} + V_{3p}^{44} + V_{3p}^{24} + V_{3p}'^{24}$$



**V7-28**

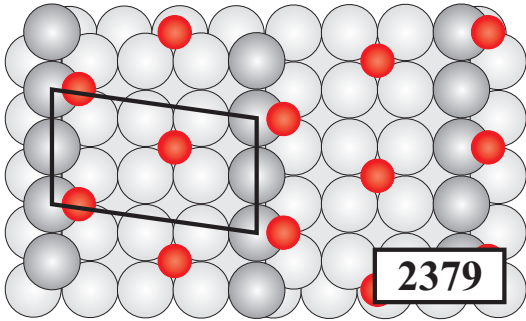
$$E_b^{V7-28} = E_{b, \text{The}}^{\text{On-site}} + E_{b, \text{Sh2}}^{\text{On-site}} + V_{3p}^{22} + V_{3p}^{44} + V_{3p}'^{24}$$





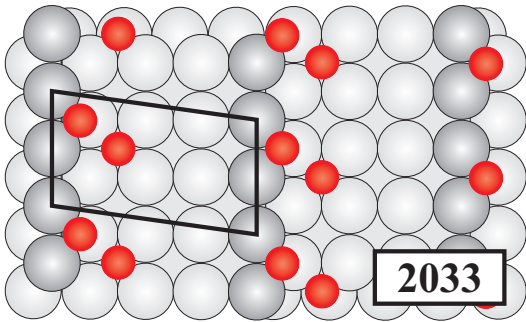
**V7-29**

$$E_b^{V7-29} = E_{b,Thc}^{On-site} + E_{b,Sh1}^{On-site} + V_{3p}^{22} + V_{3p}^{25} + V_{3p}^{55}$$



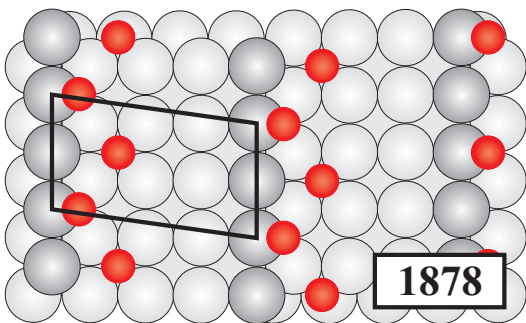
**V7-30**

$$E_b^{V7-30} = E_{b,Thc}^{On-site} + E_{b,Sh1}^{On-site} + V_{3p}^{22} + V_{3p}^{55}$$



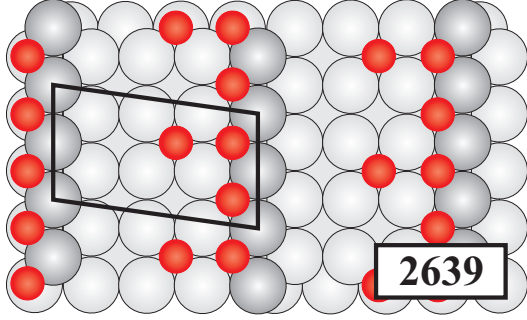
**V7-31**

$$E_b^{V7-31} = E_{b,Thl}^{On-site} + E_{b,Sh2}^{On-site} + V_{2p}^{34} + V_{3p}^{33} + V_{3p}^{34} + V_{3p}^{44}$$

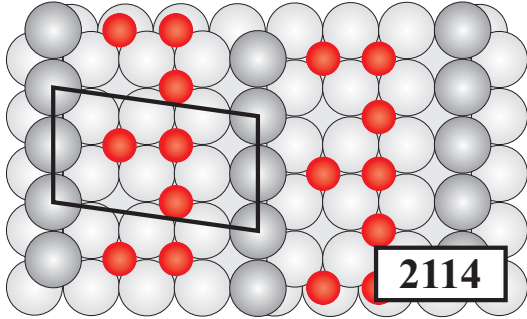


**V7-32**

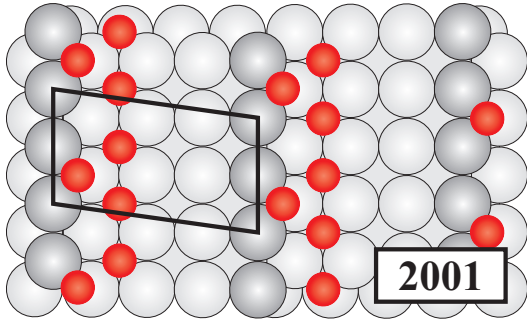
$$E_b^{V7-32} = E_{b,Thl}^{On-site} + E_{b,Sh1}^{On-site} + 2V_{2p}^{35} + V_{3p}^{33} + V_{3p}^{55}$$


**V7-33**

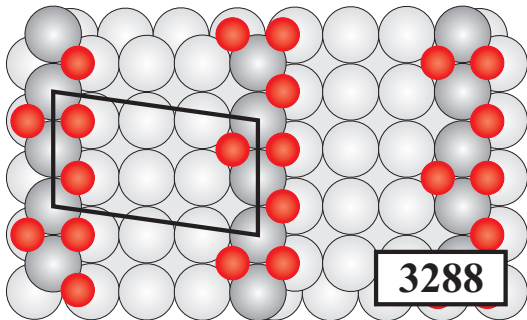
$$\begin{aligned}
 E_b^{V7-33} = & 2E_{b,Thu}^{\text{On-site}} + E_{b,Thc}^{\text{On-site}} + 2V_{1p}^{11} + 2V_{3p}^{11} \\
 & + V_{3p}^{22} + V_{1p}^{12} + 2V_{2p}^{12} + 2V_{1t}^{111} \\
 & + 2V_{2t}^{112} + 2V_{3t}^{112}
 \end{aligned}$$


**V7-34**

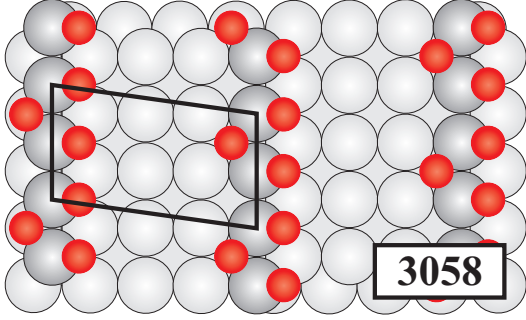
$$\begin{aligned}
 E_b^{V7-34} = & 2E_{b,Thc}^{\text{On-site}} + E_{b,Thl}^{\text{On-site}} + 2V_{1p}^{22} + 2V_{3p}^{22} \\
 & + V_{3p}^{33} + V_{1p}^{23} + 2V_{2p}^{23} + 2V_{1t}^{222} + 2V_{2t}^{223} \\
 & + 2V_{3t}^{223}
 \end{aligned}$$


**V7-35**

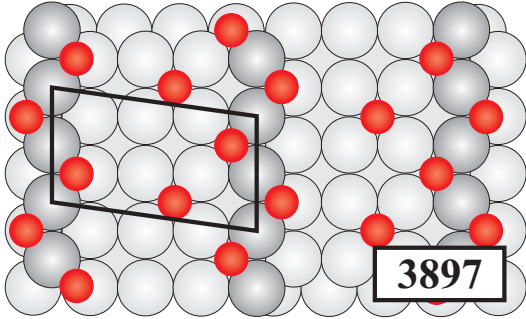
$$\begin{aligned}
 E_b^{V7-35} = & 2E_{b,Thl}^{\text{On-site}} + E_{b,Sh2}^{\text{On-site}} + 2V_{1p}^{33} + 2V_{2p}^{34} \\
 & + 2V_{3p}^{33} + 2V_{3p}^{34} + V_{3p}^{44} \\
 & + 2V_{1t}^{333} + V_{2t}^{334} + 2V_{3t}^{334}
 \end{aligned}$$


**V7-36**

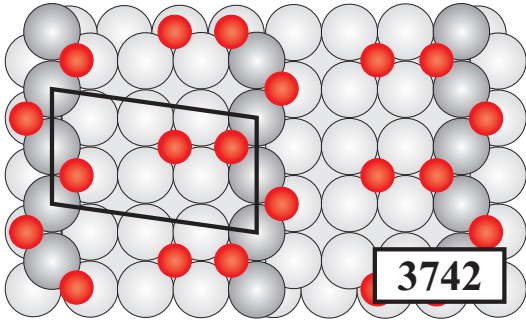
$$\begin{aligned}
 E_b^{V7-36} = & 2E_{b,Sh2}^{\text{On-site}} + E_{b,Thu}^{\text{On-site}} + 2V_{1p}^{44} + 2V_{3p}^{44} \\
 & + V_{3p}^{11} + V_{1p}^{14} + 2V_{2p}^{14} \\
 & + 2V_{1t}^{444} + 2V_{2t}^{144} + 2V_{3t}^{144}
 \end{aligned}$$


**V7-37**

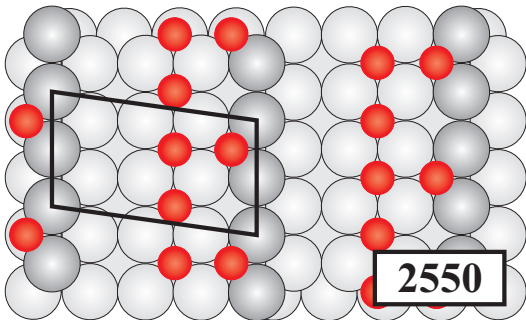
$$\begin{aligned}
 E_b^{V7-37} = & 2E_{b,Sh1}^{On-site} + E_{b,Thu}^{On-site} + 2V_{1p}^{55} + V_{3p}^{11} \\
 & + 2V_{3p}^{55} + 2V_{2p}^{15} + 2V_{3p}^{15} \\
 & + 2V_{1t}^{555} + V_{2t}^{155} + 2V_{3t}^{155}
 \end{aligned}$$


**V7-38**

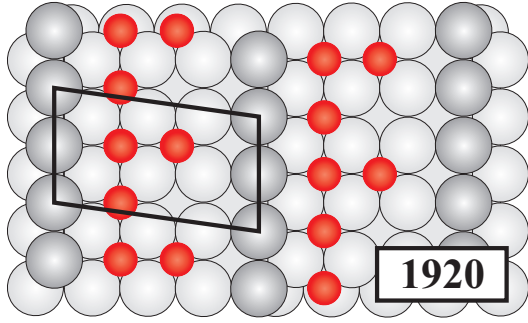
$$\begin{aligned}
 E_b^{V7-38} = & E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + E_{b,Sh2}^{On-site} \\
 & + V_{3p}^{11} + V_{3p}^{22} + V_{3p}^{44} \\
 & + 2V_{2p}^{12} + 2V_{2p}^{14} + V_{3p}^{24} + V_{3p}^{24}
 \end{aligned}$$


**V7-39**

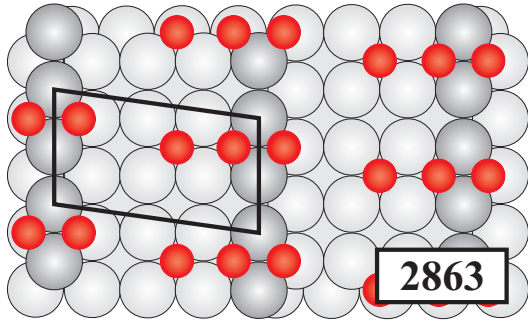
$$\begin{aligned}
 E_b^{V7-39} = & E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + E_{b,Sh2}^{On-site} \\
 & + V_{3p}^{11} + V_{3p}^{22} + V_{3p}^{44} \\
 & + V_{1p}^{12} + 2V_{2p}^{14} + V_{3p}^{24} + 2V_{3t}^{124}
 \end{aligned}$$


**V7-40**

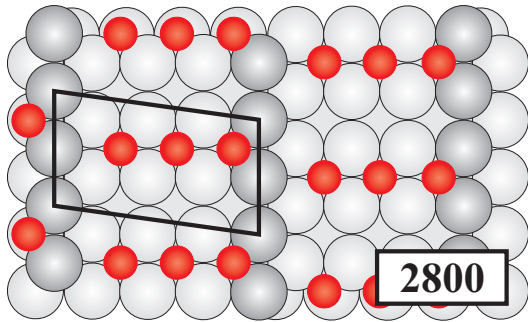
$$\begin{aligned}
 E_b^{V7-40} = & E_{b,Thu}^{On-site} + 2E_{b,Thc}^{On-site} + V_{3p}^{11} \\
 & + 2V_{1p}^{22} + 2V_{3p}^{22} + V_{1p}^{12} + 2V_{2p}^{12} \\
 & + 2V_{1t}^{222} + 2V_{2t}^{122} + 2V_{3t}^{122}
 \end{aligned}$$


**V7-41**

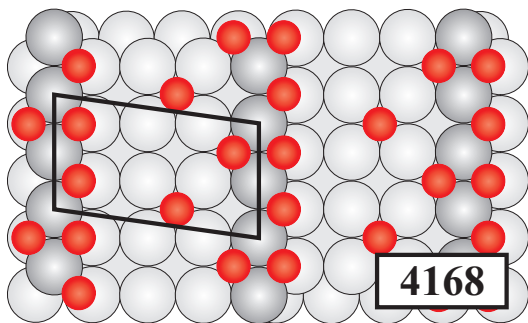
$$\begin{aligned}
 E_b^{V7-41} = & E_{b,Thc}^{On-site} + 2E_{b,Thl}^{On-site} + V_{3p}^{22} \\
 & + 2V_{1p}^{33} + 2V_{3p}^{33} + V_{1p}^{23} + 2V_{2p}^{23} \\
 & + 2V_{1t}^{333} + 2V_{2t}^{233} + 2V_{3t}^{233}
 \end{aligned}$$


**V7-42**

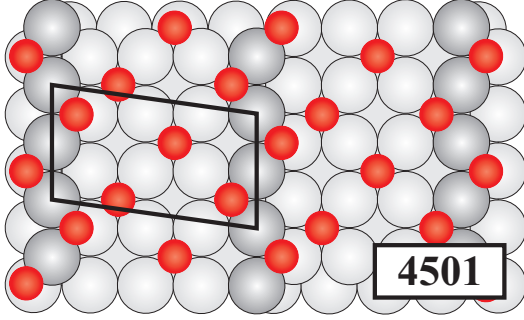
$$\begin{aligned}
 E_b^{V7-42} = & E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + E_{b,Sh2}^{On-site} \\
 & + V_{3p}^{11} + V_{3p}^{22} + V_{3p}^{44} \\
 & + V_{1p}^{12} + V_{1p}^{14} + V_{3p}^{24} + V_{3p}^{24} + V_{1t}^{124}
 \end{aligned}$$


**V7-43**

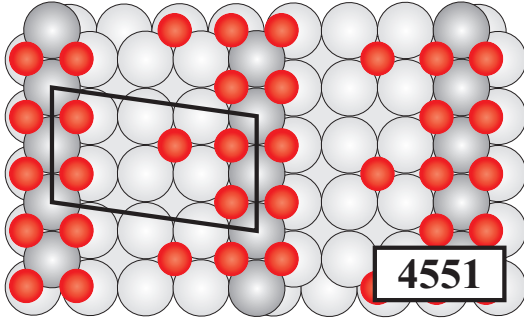
$$\begin{aligned}
 E_b^{V7-43} = & E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + E_{b,Thl}^{On-site} \\
 & + V_{3p}^{11} + V_{3p}^{22} + V_{3p}^{33} \\
 & + V_{1p}^{12} + V_{3p}^{13} + V_{3cp}^{13} + V_{1p}^{23} + V_{1t}^{123}
 \end{aligned}$$


**V7-44**

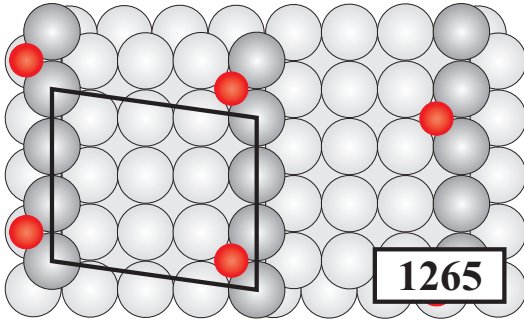
$$\begin{aligned}
 E_b^{V7-44} = & E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + 2E_{b,Sh2}^{On-site} + V_{3p}^{11} \\
 & + V_{3p}^{22} + 2V_{1p}^{44} + 2V_{3p}^{44} + V_{1p}^{14} + 2V_{2p}^{12} \\
 & + 2V_{2p}^{14} + V_{3p}^{24} + 2V_{3p}^{24} \\
 & + 2V_{1t}^{444} + 2V_{2t}^{144} + 2V_{3t}^{144} + 2V_{3t}^{124}
 \end{aligned}$$


**V7-45**

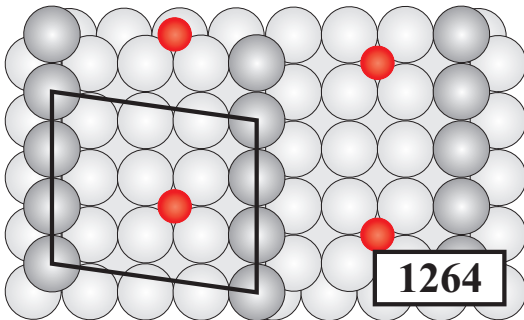
$$\begin{aligned}
 E_b^{V7-45} = & E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + E_{b,Thl}^{On-site} + E_{b,Sh2}^{On-site} \\
 & + V_{3p}^{11} + V_{3p}^{22} + V_{3p}^{33} + V_{3p}^{44} + 2V_{2p}^{12} + 2V_{2p}^{14} \\
 & + V_{1p}^{13} + V_{3cp}^{13} + 2V_{2p}^{23} + V_{3p}^{24} + V_{3p}'^{24} \\
 & + V_{2p}^{34} + V_{3p}^{34} + V_{3t}'^{134}
 \end{aligned}$$


**V7-46**

$$\begin{aligned}
 E_b^{V7-46} = & 2E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + 2E_{b,Sh2}^{On-site} + 2V_{1p}^{11} \\
 & + 2V_{3p}^{11} + V_{3p}^{22} + 2V_{1p}^{44} + 2V_{3p}^{44} + V_{1p}^{12} + 2V_{2p}^{12} \\
 & + 2V_{1p}^{14} + 4V_{2p}^{14} + V_{3p}^{24} + 2V_{3p}'^{24} + 2V_{1t}^{111} \\
 & + 2V_{2t}^{112} + 4V_{2t}^{114} + 4V_{2t}^{144} + 2V_{1t}^{444} \\
 & + V_{1t}^{124} + 2V_{3t}^{122} + 4V_{3t}^{114} + 4V_{3t}^{144} \\
 & + 2V_{3t}^{124} + 2V_{3t}'^{124}
 \end{aligned}$$

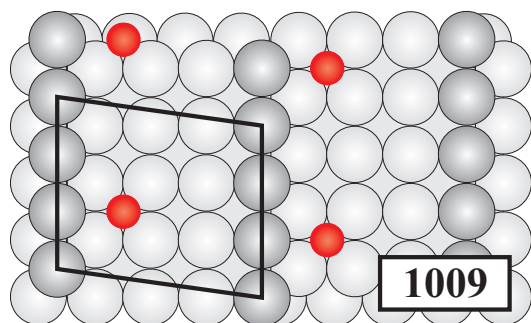

**V7-47**

$$E_b^{V7-47} = E_{b,Thu}^{On-site}$$


**V7-48**

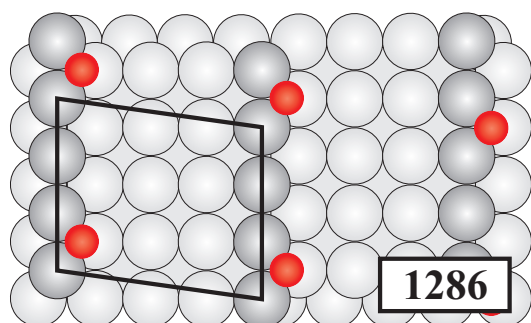
$$E_b^{V7-48} = E_{b,Thc}^{On-site}$$





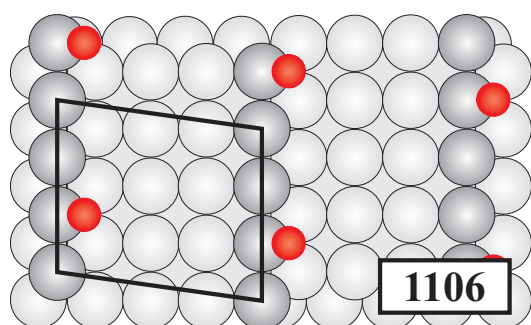
**V7-49**

$$E_b^{V7-49} = E_{b,Th1}^{On-site}$$



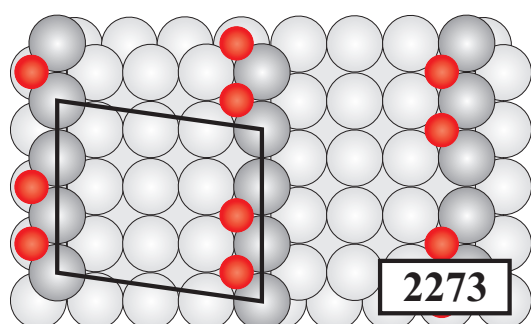
**V7-50**

$$E_b^{V7-50} = E_{b,Sh2}^{On-site}$$



**V7-51**

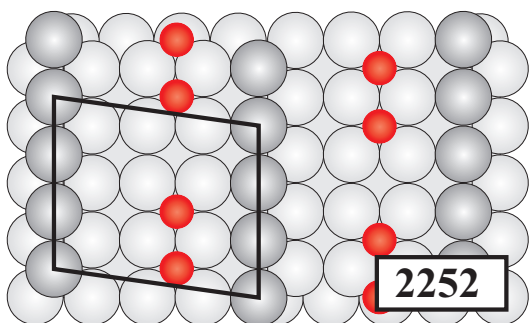
$$E_b^{V7-51} = E_{b,Sh1}^{On-site}$$



**V7-52**

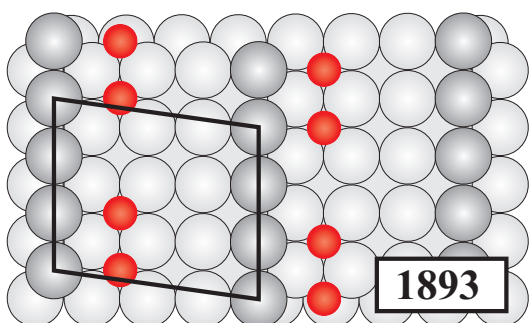
$$E_b^{V7-52} = E_{b,Thu}^{On-site} + V_{1p}^{11} + V_{3p}^{11}$$





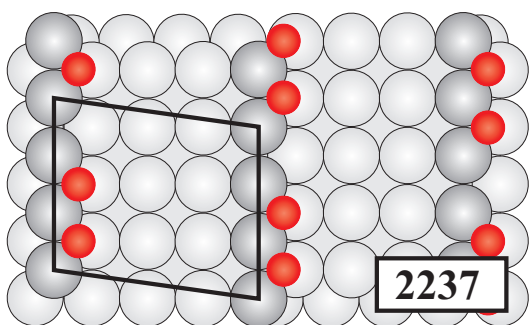
**V7-53**

$$E_b^{V7-53} = E_{b,\text{The}}^{\text{On-site}} + V_{1p}^{22} + V_{3p}^{22}$$



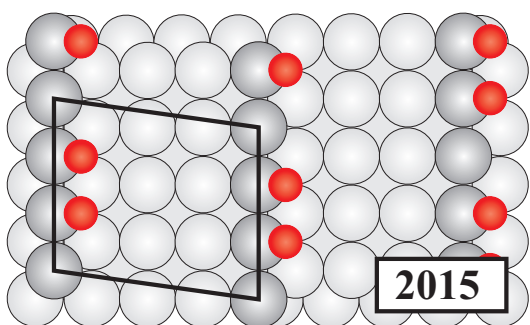
**V7-54**

$$E_b^{V7-54} = E_{b,\text{Thl}}^{\text{On-site}} + V_{1p}^{33} + V_{3p}^{33}$$



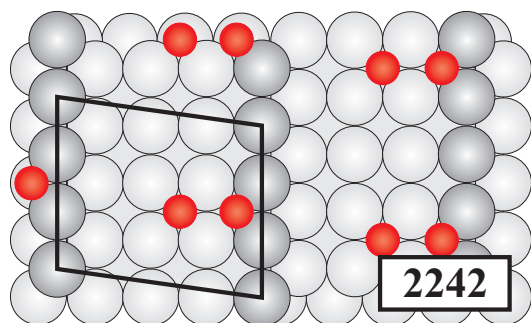
**V7-55**

$$E_b^{V7-55} = E_{b,\text{Sh2}}^{\text{On-site}} + V_{1p}^{44} + V_{3p}^{44}$$

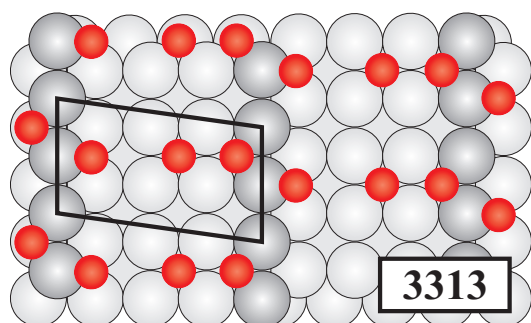


**V7-56**

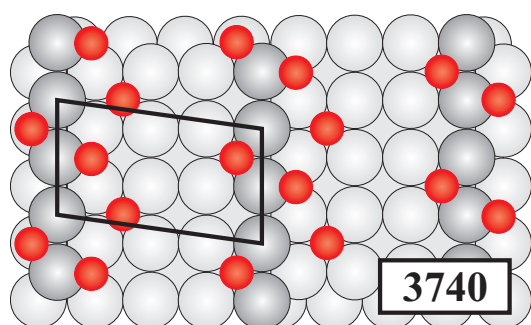
$$E_b^{V7-56} = E_{b,\text{Sh1}}^{\text{On-site}} + V_{1p}^{55} + V_{3p}^{55}$$


**V7-57**

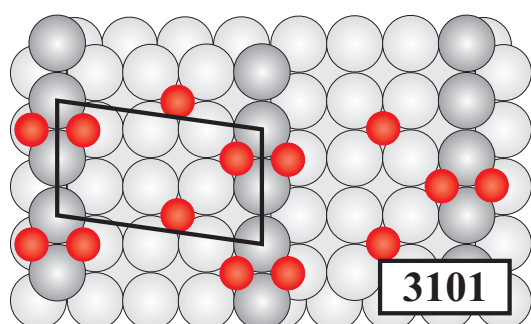
$$E_b^{V7-57} = E_{b,Thu}^{\text{On-site}} + E_{b,Thc}^{\text{On-site}} + V_{1p}^{12}$$


**V7-58**

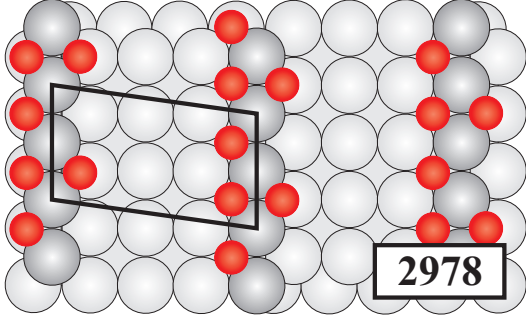
$$E_b^{V7-58} = E_{b,Thu}^{\text{On-site}} + E_{b,Thc}^{\text{On-site}} + E_{b,Sh1}^{\text{On-site}} + V_{1p}^{12} + V_{2p}^{15} \\ + V_{3p}^{11} + V_{3p}^{15} + V_{3p}^{22} + V_{3p}^{25} + V_{3p}^{55} \\ + V_{3t}^{125}$$


**V7-59**

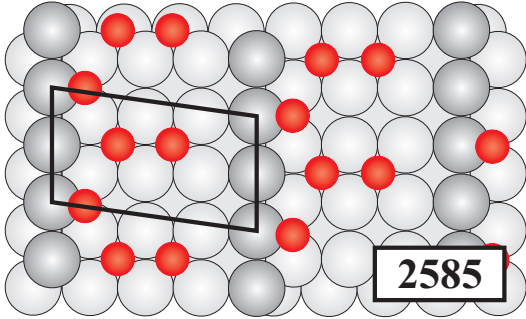
$$E_b^{V7-59} = E_{b,Thu}^{\text{On-site}} + E_{b,Thc}^{\text{On-site}} + E_{b,Sh1}^{\text{On-site}} + V_{2p}^{15} \\ + V_{3p}^{11} + V_{3cp}^{13} + V_{3p}^{15} + 2V_{2p}^{35} + V_{3p}^{33} + V_{3p}^{55} \\ + V_{3t}^{135}$$


**V7-60**

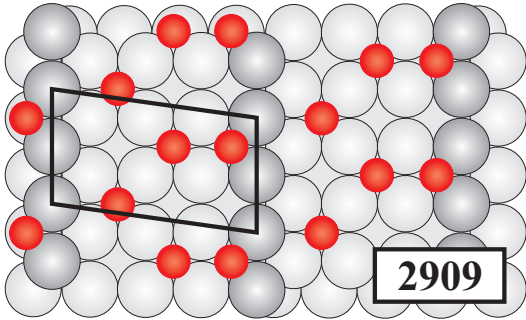
$$E_b^{V7-60} = E_{b,Thu}^{\text{On-site}} + E_{b,Thl}^{\text{On-site}} + E_{b,Sh2}^{\text{On-site}} + V_{1p}^{14} \\ + 2V_{2p}^{12} + V_{3p}^{11} + V_{3p}^{22} + V_{3p}^{24} + V_{3p}^{44} \\ + 2V_{3t}^{124}$$


**V7-61**

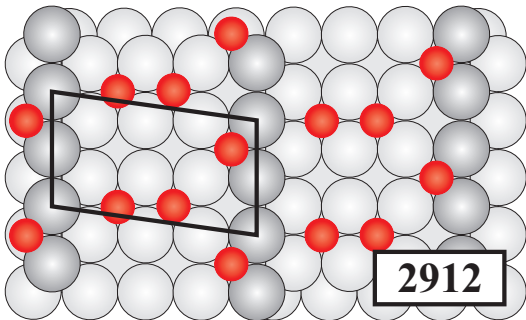
$$\begin{aligned}
 E_b^{V7-61} = & 2E_{b,Thu}^{On-site} + E_{b,Sh2}^{On-site} + 2V_{1p}^{11} + V_{1p}^{14} \\
 & + 2V_{2p}^{14} + 2V_{3p}^{11} + V_{3p}^{44} + 2V_{1t}^{111} \\
 & + 2V_{2t}^{114} + 2V_{3t}^{114}
 \end{aligned}$$


**V7-62**

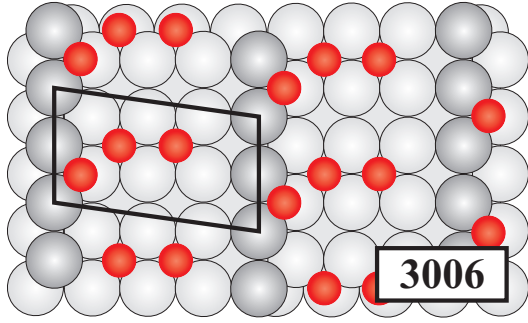
$$\begin{aligned}
 E_b^{V7-62} = & E_{b,Thc}^{On-site} + E_{b,Thl}^{On-site} + E_{b,Sh1}^{On-site} \\
 & + V_{1p}^{23} + V_{3p}^{22} + 2V_{2p}^{35} + V_{3p}^{33} + V_{3p}^{55} \\
 & + 2V_{3t}^{235}
 \end{aligned}$$


**V7-63**

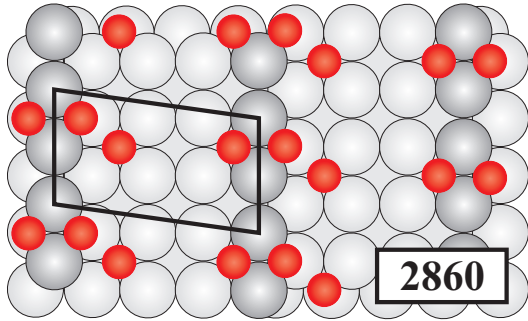
$$\begin{aligned}
 E_b^{V7-63} = & E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + E_{b,Thl}^{On-site} + V_{1p}^{12} \\
 & + V_{3p}^{11} + V_{3cp}^{13} + 2V_{2p}^{23} + V_{3p}^{22} + V_{3p}^{33} \\
 & + 2V_{3t}^{123}
 \end{aligned}$$


**V7-64**

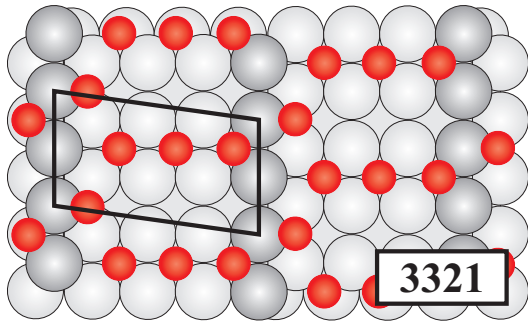
$$\begin{aligned}
 E_b^{V7-64} = & E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + E_{b,Thl}^{On-site} + 2V_{2p}^{12} \\
 & + V_{3p}^{11} + V_{3cp}^{13} + V_{1p}^{23} + V_{3p}^{22} + V_{3p}^{33} \\
 & + 2V_{3t}^{123}
 \end{aligned}$$


**V7-65**

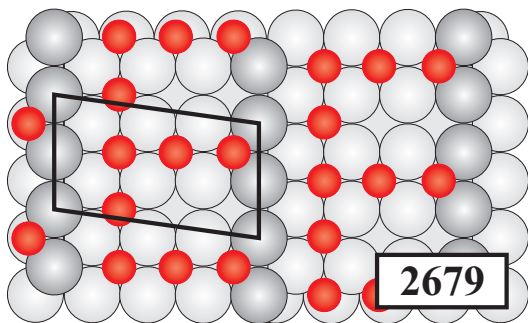
$$\begin{aligned}
 E_b^{V7-65} = & E_{b,Thc}^{On-site} + E_{b,Thl}^{On-site} + E_{b,Sh2}^{On-site} \\
 & + V_{1p}^{23} + V_{3p}^{22} + V_{3p}^{24} + V_{2p}^{34} + V_{3p}^{33} + V_{3p}^{34} \\
 & + V_{3p}^{44} + V_{3t}^{234}
 \end{aligned}$$


**V7-66**

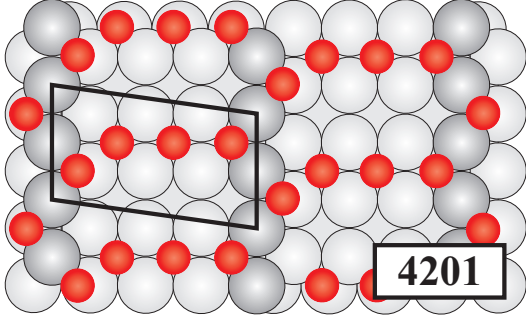
$$\begin{aligned}
 E_b^{V7-66} = & E_{b,Thu}^{On-site} + E_{b,Thl}^{On-site} + E_{b,Sh2}^{On-site} + V_{1p}^{14} \\
 & + V_{3p}^{11} + V_{3p}^{13} + V_{3cp}^{13} + V_{2p}^{34} + V_{3p}^{33} + V_{3p}^{34} \\
 & + V_{3p}^{44} + V_{3t}^{134}
 \end{aligned}$$


**V7-67**

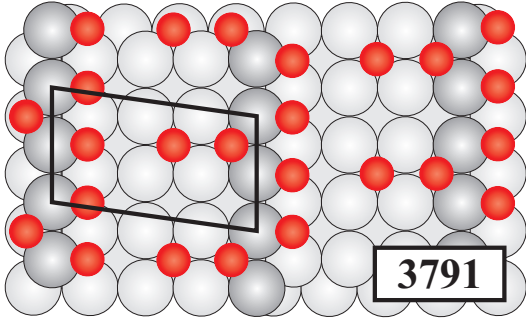
$$\begin{aligned}
 E_b^{V7-67} = & E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + E_{b,Thl}^{On-site} + E_{b,Sh1}^{On-site} \\
 & + V_{1p}^{12} + V_{2p}^{15} + V_{3p}^{11} + V_{3p}^{13} + V_{3cp}^{13} + V_{3p}^{15} + V_{1p}^{23} \\
 & + V_{3p}^{22} + 2V_{2p}^{35} + V_{3p}^{33} + V_{3p}^{55} \\
 & + V_{1t}^{123} + V_{3t}^{125} + V_{3t}^{135} + 2V_{3t}^{235}
 \end{aligned}$$


**V7-68**

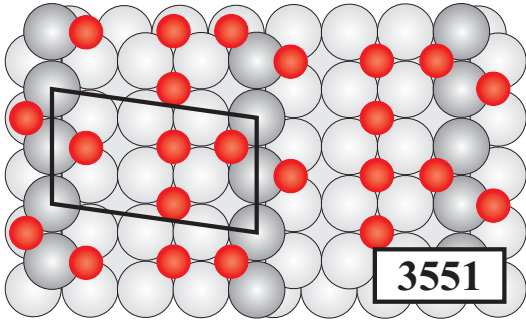
$$\begin{aligned}
 E_b^{V7-68} = & E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + 2E_{b,Thl}^{On-site} + V_{1p}^{12} \\
 & + V_{3p}^{11} + V_{3p}^{13} + 2V_{3cp}^{13} + V_{1p}^{23} + 2V_{2p}^{23} + V_{3p}^{22} \\
 & + 2V_{1p}^{33} + V_{3p}^{33} + V_{1t}^{123} + 2V_{3t}^{123} + 2V_{2t}^{233} \\
 & + 2V_{3t}^{233} + 2V_{1t}^{333}
 \end{aligned}$$


**V7-69**

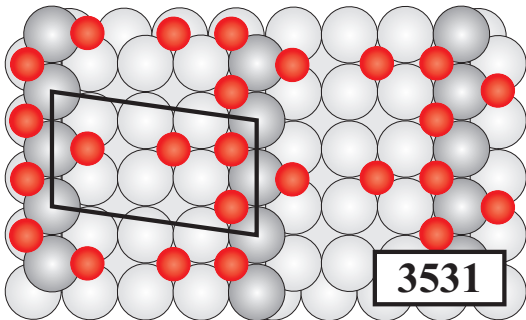
$$\begin{aligned}
 E_b^{V7-69} = & E_{b,Thu}^{\text{On-site}} + E_{b,Thc}^{\text{On-site}} + E_{b,Thl}^{\text{On-site}} + E_{b,Sh2}^{\text{On-site}} \\
 & + V_{1p}^{12} + 2V_{2p}^{14} + V_{3p}^{11} + V_{3p}^{13} + V_{3cp}^{13} + V_{1p}^{23} \\
 & + V_{3p}^{22} + V_{3p}^{24} + V_{2p}^{34} + V_{3p}^{33} + V_{3p}^{34} + V_{3p}^{44} \\
 & + V_{1t}^{123} + 2V_{3t}^{124} + V_{3t}^{134} + V_{3t}^{234}
 \end{aligned}$$


**V7-70**

$$\begin{aligned}
 E_b^{V7-70} = & E_{b,Thu}^{\text{On-site}} + E_{b,Thc}^{\text{On-site}} + 2E_{b,Sh1}^{\text{On-site}} + V_{1p}^{12} \\
 & + 2V_{2p}^{15} + V_{3p}^{11} + 2V_{3p}^{15} + V_{3p}^{22} + V_{3p}^{25} \\
 & + 2V_{1p}^{55} + 2V_{3p}^{55} + V_{2t}^{155} + 2V_{3t}^{155} + 2V_{3t}^{125} \\
 & + 2V_{1t}^{555}
 \end{aligned}$$

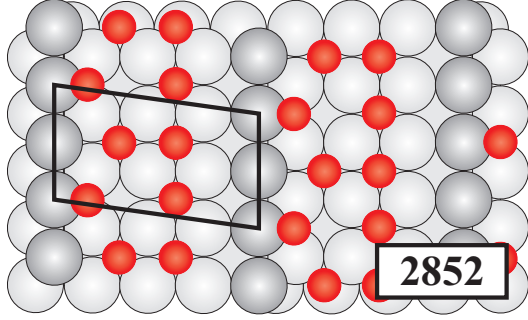

**V7-71**

$$\begin{aligned}
 E_b^{V7-71} = & E_{b,Thu}^{\text{On-site}} + 2E_{b,Thc}^{\text{On-site}} + E_{b,Sh1}^{\text{On-site}} + V_{1p}^{12} \\
 & + 2V_{2p}^{12} + V_{2p}^{15} + V_{3p}^{11} + V_{3p}^{15} + 2V_{1p}^{22} + 2V_{3p}^{22} \\
 & + V_{3p}^{25} + V_{3p}^{55} + 2V_{2t}^{122} + 2V_{3t}^{122} + V_{3t}^{125} \\
 & + 2V_{1t}^{222}
 \end{aligned}$$

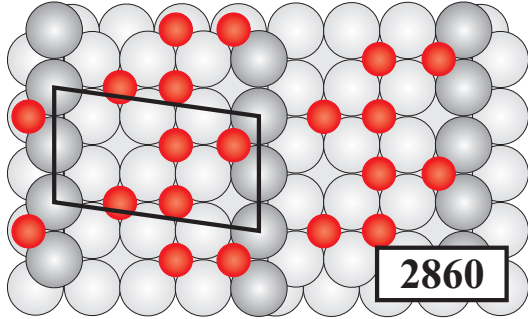

**V7-72**

$$\begin{aligned}
 E_b^{V7-72} = & 2E_{b,Thu}^{\text{On-site}} + E_{b,Thc}^{\text{On-site}} + E_{b,Sh1}^{\text{On-site}} + 2V_{1p}^{11} \\
 & + V_{1p}^{12} + 2V_{2p}^{12} + 2V_{2p}^{15} + 2V_{3p}^{11} + 2V_{3p}^{15} + V_{3p}^{22} \\
 & + V_{3p}^{25} + V_{3p}^{55} + 2V_{1t}^{111} + 2V_{2t}^{112} + V_{2t}^{115} + 2V_{3t}^{112} \\
 & + 2V_{3t}^{115} + V_{3t}^{125}
 \end{aligned}$$

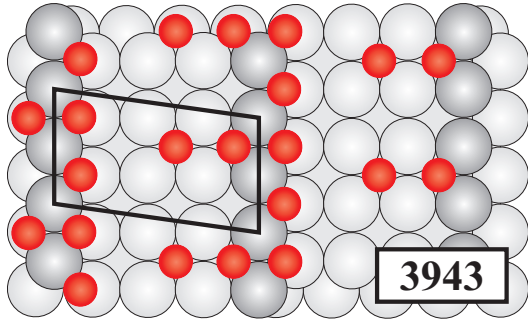



**V7-73**

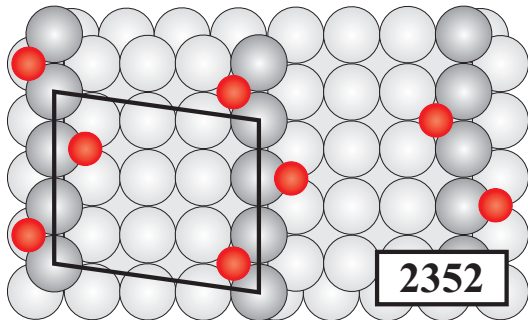
$$\begin{aligned}
 E_b^{V7-73} = & 2E_{b,Thc}^{On-site} + E_{b,Thl}^{On-site} + E_{b,Sh1}^{On-site} + 2V_{1p}^{22} \\
 & + V_{1p}^{23} + 2V_{2p}^{23} + 2V_{3p}^{22} + V_{3p}^{25} + 2V_{3p}^{35} \\
 & + V_{3p}^{33} + V_{3p}^{55} + 2V_{1t}^{222} + 2V_{2t}^{223} + 2V_{3t}^{223} \\
 & + 2V_{3t}^{235}
 \end{aligned}$$


**V7-74**

$$\begin{aligned}
 E_b^{V7-74} = & E_{b,Thu}^{On-site} + 2E_{b,Thc}^{On-site} + E_{b,Thl}^{On-site} + V_{1p}^{12} \\
 & + 2V_{2p}^{12} + V_{3p}^{11} + V_{3p}^{13} + 2V_{1p}^{22} + V_{1p}^{23} + 2V_{2p}^{23} \\
 & + 2V_{3p}^{22} + 2V_{2t}^{122} + 2V_{3t}^{122} + 2V_{3t}^{123} \\
 & + 2V_{3t}^{123} + 2V_{1t}^{222} + 2V_{2t}^{223} + 2V_{3t}^{223}
 \end{aligned}$$

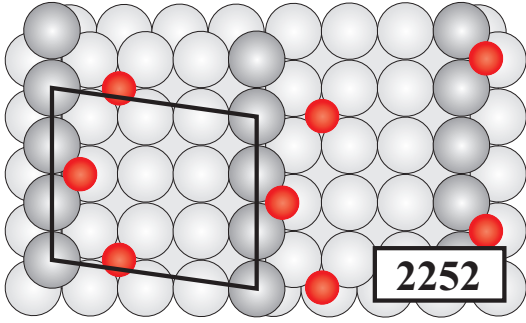

**V7-75**

$$\begin{aligned}
 E_b^{V7-75} = & E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + 2E_{b,Sh2}^{On-site} + V_{1p}^{12} \\
 & + V_{1p}^{14} + 2V_{2p}^{14} + V_{3p}^{11} + V_{3p}^{22} + V_{3p}^{24} + 2V_{3p}^{24} \\
 & + 2V_{1p}^{44} + 2V_{3p}^{44} + V_{1t}^{124} + 2V_{2t}^{144} + 2V_{3t}^{144} \\
 & + 2V_{3t}^{124} + 2V_{1t}^{444}
 \end{aligned}$$


**V7-76**

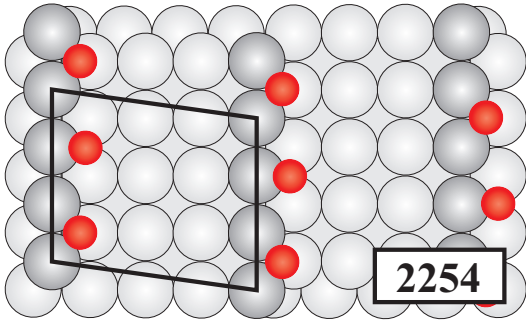
$$\begin{aligned}
 E_b^{V7-76} = & E_{b,Thu}^{On-site} + E_{b,Sh1}^{On-site} \\
 & + 2V_{3p}^{15}
 \end{aligned}$$





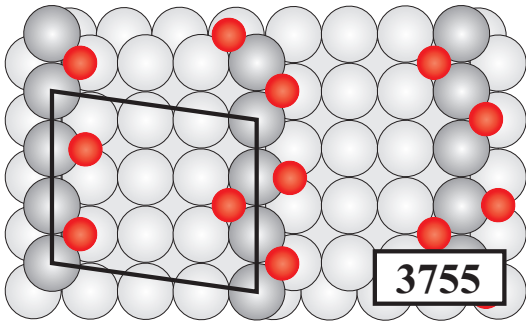
**V7-77**

$$E_b^{V7-77} = E_{b,Th1}^{On-site} + E_{b,Sh2}^{On-site} + 2V_{3p}^{34}$$



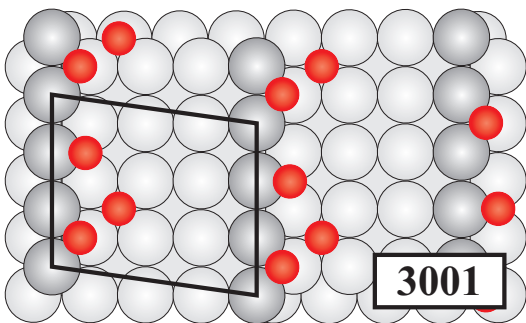
**V7-78**

$$E_b^{V7-78} = E_{b,Sh1}^{On-site} + E_{b,Sh2}^{On-site} + 2V_{3p}^{45}$$



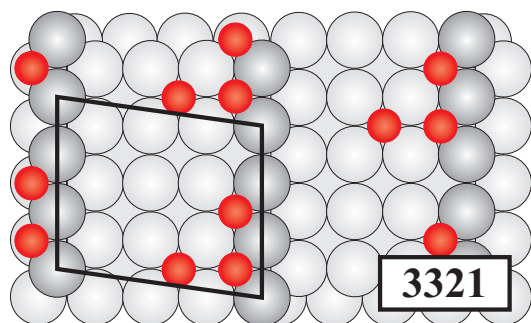
**V7-79**

$$E_b^{V7-79} = E_{b,Thu}^{On-site} + E_{b,Sh1}^{On-site} + E_{b,Sh2}^{On-site} + V_{2p}^{14} + V_{2p}^{15} + 2V_{3p}^{45} + V_{3t}^{145}$$



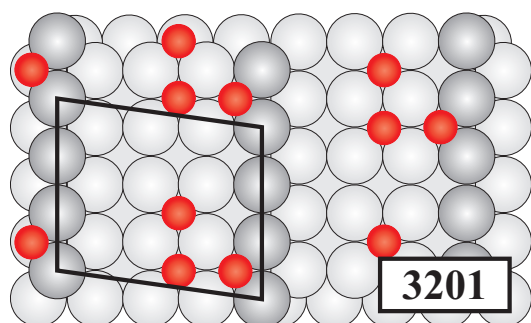
**V7-80**

$$E_b^{V7-80} = E_{b,Th1}^{On-site} + E_{b,Sh1}^{On-site} + E_{b,Sh2}^{On-site} + V_{2p}^{34} + V_{2p}^{35} + 2V_{3p}^{45} + V_{3t}^{345}$$



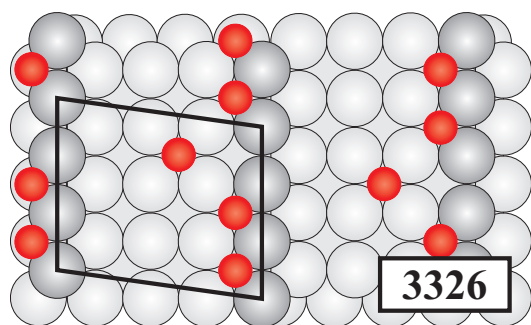
**V7-81**

$$E_b^{V7-81} = 2E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + V_{1p}^{11} + V_{1p}^{12} + V_{2p}^{12} + V_{3p}^{11} + V_{2t}^{112}$$



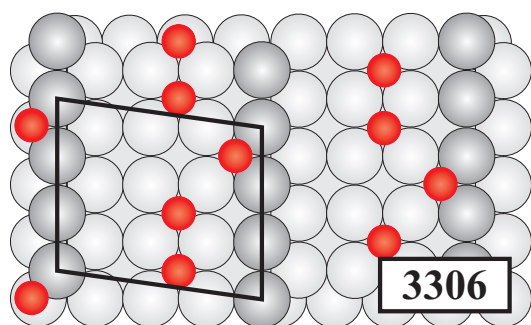
**V7-82**

$$E_b^{V7-82} = E_{b,Thu}^{On-site} + 2E_{b,Thc}^{On-site} + V_{1p}^{12} + V_{1p}^{22} + V_{2p}^{12} + V_{3p}^{22} + V_{2t}^{122}$$



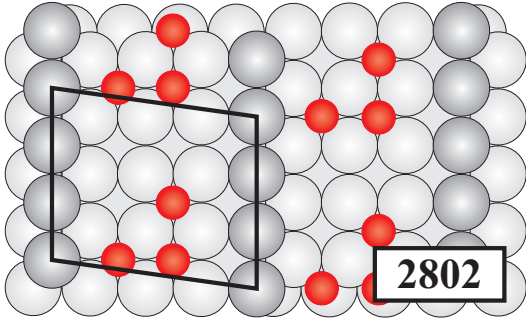
**V7-83**

$$E_b^{V7-83} = 2E_{b,Thu}^{On-site} + E_{b,Thc}^{On-site} + V_{1p}^{11} + 2V_{2p}^{12} + V_{3p}^{11} + 2V_{3t}^{112}$$

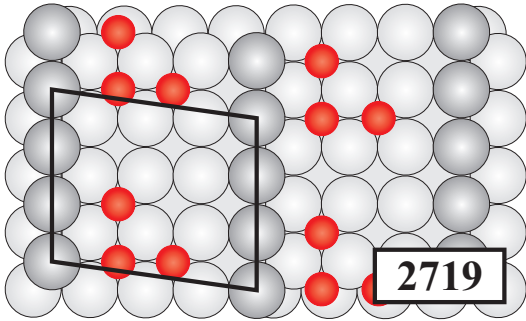


**V7-84**

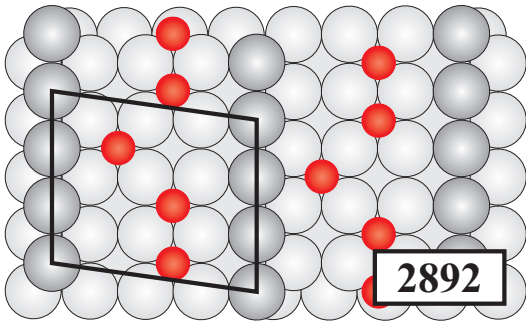
$$E_b^{V7-84} = E_{b,Thu}^{On-site} + 2E_{b,Thc}^{On-site} + V_{1p}^{22} + 2V_{2p}^{12} + V_{3p}^{22} + 2V_{3t}^{122}$$


**V7-85**

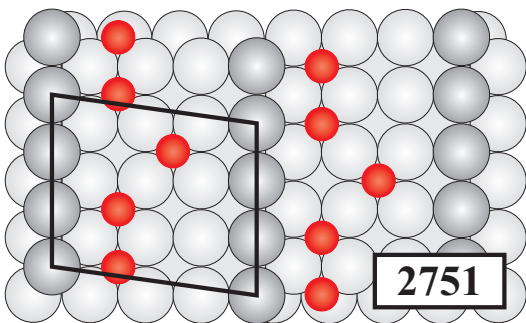
$$E_b^{V7-85} = 2E_{b,Thc}^{On-site} + E_{b,Thl}^{On-site} + V_{1p}^{22} + V_{1p}^{23} + V_{2p}^{23} + V_{3p}^{22} + V_{2t}^{223}$$


**V7-86**

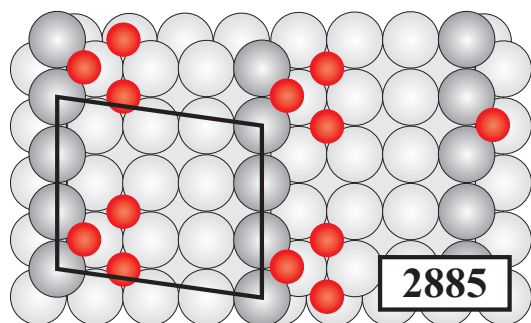
$$E_b^{V7-86} = E_{b,Thc}^{On-site} + 2E_{b,Thl}^{On-site} + V_{1p}^{23} + V_{2p}^{23} + V_{1p}^{33} + V_{3p}^{33} + V_{2t}^{233}$$


**V7-87**

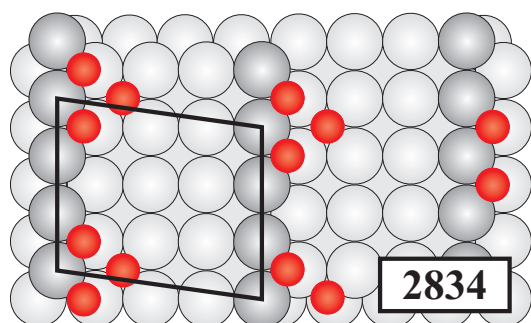
$$E_b^{V7-87} = 2E_{b,Thc}^{On-site} + E_{b,Thl}^{On-site} + V_{1p}^{22} + 2V_{2p}^{23} + V_{3p}^{22} + 2V_{3t}^{223}$$


**V7-88**

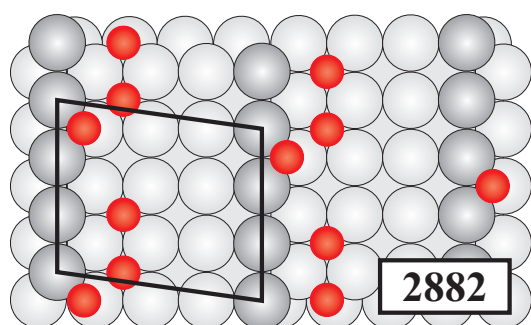
$$E_b^{V7-88} = E_{b,Thc}^{On-site} + 2E_{b,Thl}^{On-site} + 2V_{2p}^{23} + V_{1p}^{33} + V_{3p}^{33} + 2V_{3t}^{233}$$


**V7-89**

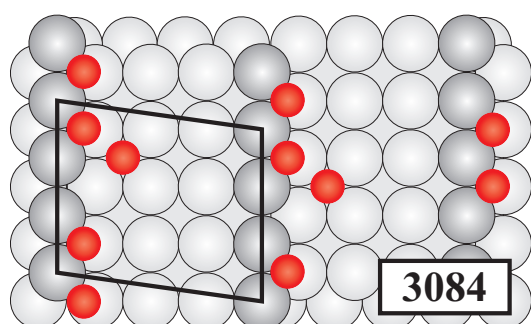
$$E_b^{V7-89} = 2E_{b,Thl}^{On-site} + E_{b,Sh2}^{On-site} + V_{1p}^{33} + 2V_{2p}^{34} + V_{3p}^{33} + V_{2t}^{334}$$


**V7-90**

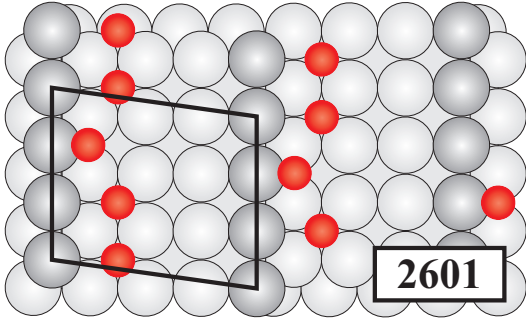
$$E_b^{V7-90} = E_{b,Thl}^{On-site} + 2E_{b,Sh2}^{On-site} + 2V_{2p}^{34} + V_{1p}^{44} + V_{3p}^{44} + V_{2t}^{344}$$


**V7-91**

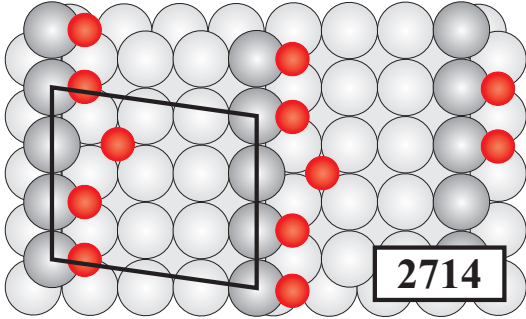
$$E_b^{V7-91} = 2E_{b,Thl}^{On-site} + E_{b,Sh2}^{On-site} + V_{1p}^{33} + V_{2p}^{34} + V_{3p}^{33} + 2V_{3p}^{34} + V_{3t}^{334}$$


**V7-92**

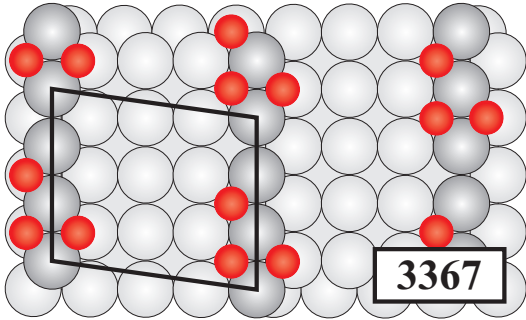
$$E_b^{V7-92} = E_{b,Thl}^{On-site} + 2E_{b,Sh2}^{On-site} + V_{2p}^{34} + 2V_{3p}^{34} + V_{1p}^{44} + V_{3p}^{44} + V_{3t}^{344}$$


**V7-93**

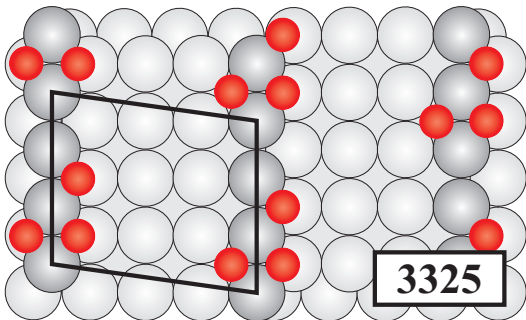
$$E_b^{V7-93} = 2E_{b,Thl}^{On-site} + E_{b,Sh1}^{On-site} + V_{1p}^{33} + 2V_{2p}^{35} + V_{3p}^{33} + 2V_{3t}^{335}$$


**V7-94**

$$E_b^{V7-94} = E_{b,Thl}^{On-site} + 2E_{b,Sh1}^{On-site} + 2V_{2p}^{35} + V_{1p}^{55} + V_{3p}^{55} + 2V_{3t}^{355}$$

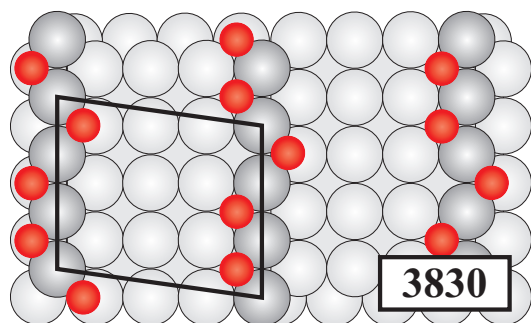

**V7-95**

$$E_b^{V7-95} = 2E_{b,Thu}^{On-site} + E_{b,Sh2}^{On-site} + V_{1p}^{11} + V_{1p}^{14} + V_{2p}^{14} + V_{3p}^{11} + V_{3t}^{335}$$


**V7-96**

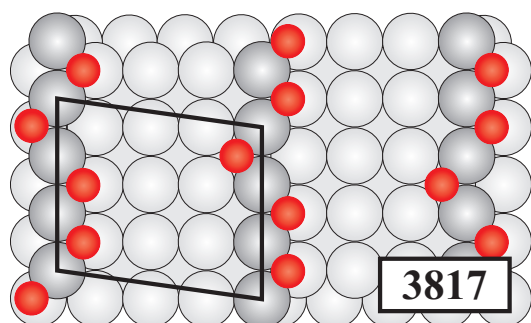
$$E_b^{V7-96} = E_{b,Thu}^{On-site} + 2E_{b,Sh2}^{On-site} + V_{1p}^{14} + V_{2p}^{14} + V_{1p}^{44} + V_{3p}^{44} + V_{2t}^{144}$$





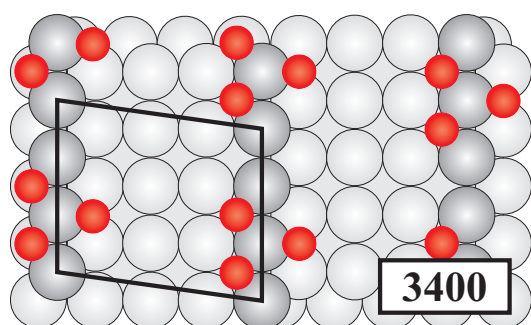
**V7-97**

$$E_b^{V7-96} = 2E_{b,Thu}^{On-site} + E_{b,Sh2}^{On-site} + V_{1p}^{11} + 2V_{2p}^{14} + V_{3p}^{11} + 2V_{3t}^{114}$$



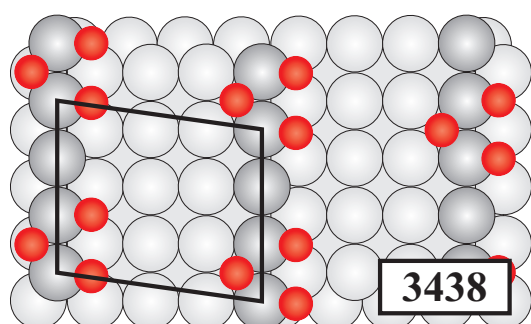
**V7-98**

$$E_b^{V7-98} = E_{b,Thu}^{On-site} + 2E_{b,Sh2}^{On-site} + 2V_{2p}^{14} + V_{1p}^{44} + V_{3p}^{44} + 2V_{3t}^{144}$$



**V7-99**

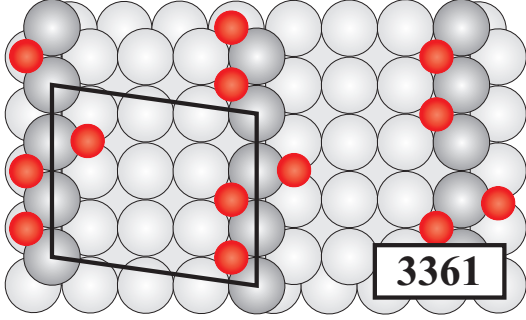
$$E_b^{V7-99} = 2E_{b,Thu}^{On-site} + E_{b,Sh1}^{On-site} + V_{1p}^{11} + 2V_{2p}^{15} + V_{3p}^{11} + V_{2t}^{115}$$



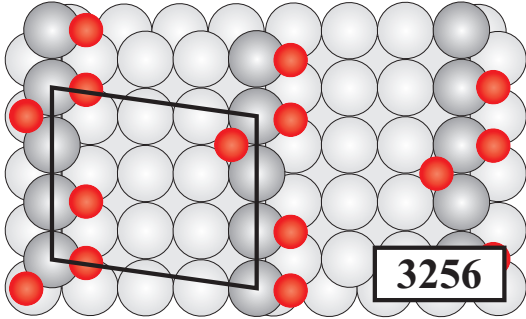
**V7-100**

$$E_b^{V7-100} = E_{b,Thu}^{On-site} + 2E_{b,Sh1}^{On-site} + 2V_{2p}^{15} + V_{1p}^{55} + V_{3p}^{55} + V_{2t}^{155}$$

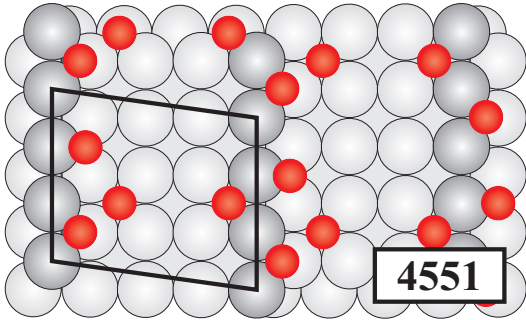



**V7-101**

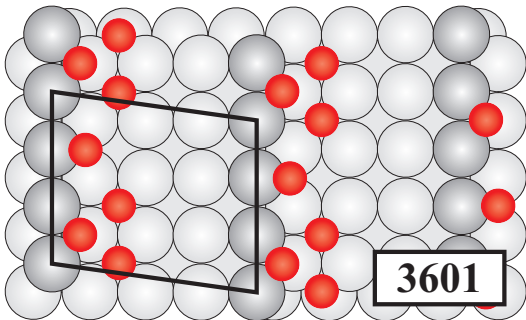
$$E_b^{V7-101} = 2E_{b,Thu}^{On-site} + E_{b,Sh1}^{On-site} + V_{1p}^{11} + V_{2p}^{15} + V_{3p}^{11} + 2V_{3p}^{15} + V_{3t}^{115}$$


**V7-102**

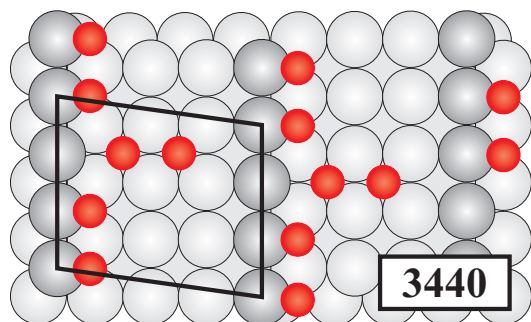
$$E_b^{V7-102} = E_{b,Thu}^{On-site} + 2E_{b,Sh1}^{On-site} + V_{2p}^{15} + V_{1p}^{55} + V_{3p}^{55} + 2V_{3p}^{15} + V_{3t}^{155}$$


**V7-103**

$$E_b^{V7-103} = E_{b,Thu}^{On-site} + E_{b,Thl}^{On-site} + E_{b,Sh2}^{On-site} + E_{b,Sh1}^{On-site} + V_{2p}^{14} + V_{2p}^{15} + V_{3p}^{13} + V_{3cp}^{13} + V_{2p}^{34} + V_{2p}^{35} + 2V_{3p}^{45} + V_{3t}^{134} + V_{3t}^{135} + V_{3t}^{145} + V_{3t}^{345}$$


**V7-104**

$$E_b^{V7-104} = 2E_{b,Thl}^{On-site} + E_{b,Sh2}^{On-site} + E_{b,Sh1}^{On-site} + V_{1p}^{33} + 2V_{2p}^{34} + 2V_{2p}^{35} + V_{3p}^{33} + 2V_{3p}^{45} + V_{2t}^{334} + 2V_{3t}^{335} + 2V_{3t}^{345}$$



### V7-105

$$\begin{aligned}
 E_b^{V7-105} = & E_{b,Thc}^{\text{On-site}} + E_{b,Thl}^{\text{On-site}} + 2E_{b,Shl}^{\text{On-site}} \\
 & + V_{1p}^{23} + 2V_{2p}^{35} + V_{1p}^{55} + V_{3p}^{55} \\
 & + 2V_{3t}^{235} + 2V_{3t}^{355}
 \end{aligned}$$