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3d ... LDA ... 3d- ...

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 $l$ ,  $\dots$   $K$  -  $\dots$   $l$   
 $l - \dots l l l \dots$   
 $\dots l$  (F. 1. 2),  $\dots$   
 $\dots \varepsilon(q/q')$  (F. 3),  $\dots$   
 $\dots q - q'.$   $\dots q$   $\dots l$   
 $\dots$   $\dots l - \dots l$   
 $K$  -  $\dots l l$ ,  $\dots \varepsilon(q/q')$   
 $\dots$   $\dots l$   
 $\dots l l (\dots), \dots l l$   
 $\dots (\dots).$   $\dots l$   
 $\dots (l \dots) \dots \Pi$   
 $\varepsilon(q/q')$   $\dots$   $l l$   
 $K$  -  $\dots l - \dots l l l.$

72 - 80  $\dots Z O$   $\dots I_2 O_3, \dots$   $l.$   
 $l \dots \dots$  22  $l l l$   
 $\dots$  1.19  $l -$   
**!**

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 $l l$   $N$   $Z O$   $G$   $I_2 O_3$   $3d^1 - 3d^8$   
 $\dots$   $3d l \dots$   $\dots \Pi$

R. 28 29. I. 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100.

B. 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100.

LDA & GGA  $+U$  [\[18, 19\]](#)





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