

উদাহরণস্বরূপ (50-52) এর

$O(10)$ এর উদাহরণ, ফল

$$H_{LDA}(x) \equiv E_{\theta} [V(x)]$$

x			H_{CE}	H_{LDA}	H_{CE}
o 2					
1/9	A_8B	{301} A_8B	45.1...	38.5	39.4
1/6	A_5B	{301} A_5B	59.5...	55.9	57.4
1/5	A_4B	{201} & {301} A_4B	71.3...	67.9	67.3
5/12	A_7B_5	{302} $A_2B_2A_3B_2A_2B$	91.3...	89.1	93.7
o 3					
1/5	$A_{12}B_3$	{301} A_5BABA_6B	71.0...	67.9	67.5
4/15	$A_{11}B_4$	{401} A_5BABA_4BAB	86.6...	84.9	85.4
2/5	A_9B_6	{401} $A_4B_4A_4BAB$	92.9...	91.6	93.6
2/3	A_4B_8	{302} $B_5A_2B_3A_2$	69.0...	63.2	58.7
	A_2B_4	{301} A_2B_4	68.6...	66.4	59.1
o 4					
2/11	A_9B_2	{301} A_5BA_4B	64.9...	62.3	62.5
1/3	$A_{10}B_5$	{401} $A_4BABA_2BA_2BAB$	91.9...	87.8	87.8
	A_8B_4 (.4905)	{302} $A_5B_2A_3B_2$	95.7...	85.4	91.1
2/5	A_3B_2	{110} A_2BAB	94.0...	86.7	89.4
5/8	A_3B_5	{401} B_4A_2BA	75.6...	68.2	64.1
2/3	A_4B_8	{601} B_6ABA_2BA	68.2...	61.6	60.7
o 5					
1/6	$A_{10}B_2$	{ } ()	62.2...	54.2	55.3
1/5	A_8B_2	{ } ()	71.5...	66.5	66.5
1/3	A_8B_4 (.4557)	{301} $A_3BA_2BA_3B_2$	91.2...	88.8	91.1
7/12	A_5B_7	{302} $B_2A_2B_3A_2B_2A$	94.4...	91.9	74.8
o 6					
1/9	$A_{18}B_2$	{ } ()	37.9...	34.8	34.4
2/17	$A_{15}B_2$	{401} $A_{14}BAB$	43.0...	41.4	41.0
4/17	$A_{13}B_4$	{401} A_6BABA_5BAB	81.5...	78.9	79.9
1/2	A_3B_3 (.55)	{111} A_3B_3	41.3...	7.4	11.6
o 7					
1/11	$A_{10}B$	{301} $A_{10}B_1$	32.7...	31.7	31.4
2/13	$A_{11}B_2$	{301} A_6BA_5B	54.7...	53.2	53.3

I. RANGE OF INFRAC ION REQUIRED FOR DE CRIBING L_4

At L_2 () f ... of the ...
 At L_3 () f ... of the ...
 At L_4 () f ... of the ...



Fig. 11. Energy band structure of Au_2Pd_4 (left) and Au_0Pd_4 (right) calculated by LDA. The energy is in eV.

) CE ... LDA ...
 Au_2Pd_4 ...
) CE ... LDA ...
 Au_0Pd_4 ...
) S ... LDA ...
 Au_2Pd_4 ...
) ...
 Au_2Pd_4 ...

3. Generic behaviors during outer-loop iterations
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 ...
 ...

... H_{LDA} ...
 ... H_{LDA} ...
 ... H_{CE} ...
 13. ... 2.8

... $[\dots]$... 12.

II. DI CZ ION OF GRZND- A E ORDERED-
 RZC, ZINE INA $1 \times 1 \times x$

... A_1 ...
 14. ...

A. μ - $A_{1 \times 1 \times x}$ m s, x 0.22: (301) " t
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... of ...
 ... 87 ...
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 ... (001) ...
 ... A ...

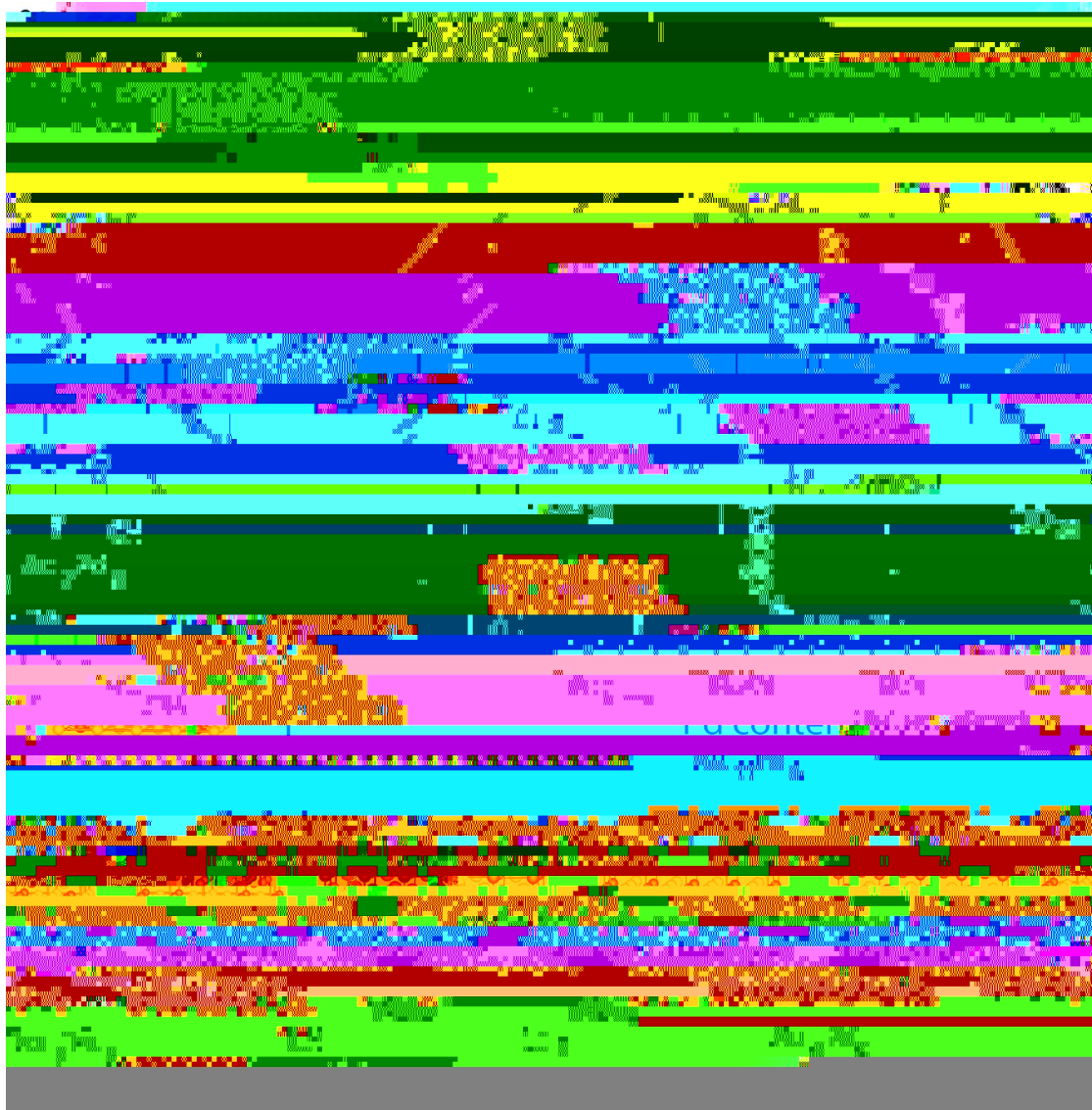


Fig. 14. (1) $\Delta z = 0.22$ (2) $\Delta z = 0.44$ (3) $\Delta z = 0.66$ (4) $\Delta z = 0.88$ (5) $\Delta z = 1.1$ (6) $\Delta z = 1.32$ (7) $\Delta z = 1.54$ (8) $\Delta z = 1.76$ (9) $\Delta z = 1.98$ (10) $\Delta z = 2.2$ (11) $\Delta z = 2.42$ (12) $\Delta z = 2.64$ (13) $\Delta z = 2.86$ (14) $\Delta z = 3.08$ (15) $\Delta z = 3.3$ (16) $\Delta z = 3.52$ (17) $\Delta z = 3.74$ (18) $\Delta z = 3.96$ (19) $\Delta z = 4.18$ (20) $\Delta z = 4.4$ (21) $\Delta z = 4.62$ (22) $\Delta z = 4.84$ (23) $\Delta z = 5.06$ (24) $\Delta z = 5.28$ (25) $\Delta z = 5.5$ (26) $\Delta z = 5.72$ (27) $\Delta z = 5.94$ (28) $\Delta z = 6.16$ (29) $\Delta z = 6.38$ (30) $\Delta z = 6.6$ (31) $\Delta z = 6.82$ (32) $\Delta z = 7.04$ (33) $\Delta z = 7.26$ (34) $\Delta z = 7.48$ (35) $\Delta z = 7.7$ (36) $\Delta z = 7.92$ (37) $\Delta z = 8.14$ (38) $\Delta z = 8.36$ (39) $\Delta z = 8.58$ (40) $\Delta z = 8.8$ (41) $\Delta z = 9.02$ (42) $\Delta z = 9.24$ (43) $\Delta z = 9.46$ (44) $\Delta z = 9.68$ (45) 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= 122.66$ (569) $\Delta z = 122.88$ (570) $\Delta z = 123$ (571) $\Delta z = 123.22$ (572) $\Delta z = 123.44$ (573) $\Delta z = 123.66$ (574) $\Delta z = 123.88$ (575) $\Delta z = 124$ (576) $\Delta z = 124.22$ (577) $\Delta z = 124.44$ (578) $\Delta z = 124.66$ (579) $\Delta z = 124.88$ (580) $\Delta z = 125$ (581) $\Delta z = 125.22$ (582) $\Delta z = 125.44$ (583) $\Delta z = 125.66$ (584) $\Delta z = 125.88$ (585) $\Delta z = 126$ (586) $\Delta z = 126.22$ (587) $\Delta z = 126.44$ (588) $\Delta z = 126.66$ (589) $\Delta z = 126.88$ (590) $\Delta z = 127$ (591) $\Delta z = 127.22$ (592) $\Delta z = 127.44$ (593) $\Delta z = 127.66$ (594) $\Delta z = 127.88$ (595) $\Delta z = 128$ (596) $\Delta z = 128.22$ (597) $\Delta z = 128.44$ (598) $\Delta z = 128.66$ (599) $\Delta z = 128.88$ (600) $\Delta z = 129$ (601) $\Delta z = 129.22$ (602) $\Delta z = 129.44$ (603) $\Delta z = 129.66$ (604) $\Delta z = 129.88$ (605) $\Delta z = 130$ (606) $\Delta z = 130.22$ (607) $\Delta z = 130.44$ (608) $\Delta z = 130.66$ (609) $\Delta z = 130.88$ (610) $\Delta z = 131$ (611) $\Delta z = 131.22$ (612) $\Delta z = 131.44$ (613) $\Delta z = 131.66$ (614) $\Delta z = 131.88$ (615) $\Delta z = 132$ (616) $\Delta z = 132.22$ (617) $\Delta z = 13$

$N_0 = 176$
 $3 \cdot 10^6$
 $x = 1/3$
 $C37$
 A_3
 $L1_2$
 $H_{LDA}(C37)$
 $C37$
 $C37$
 A_3
 $D0_3$
 A_3
 $H_{LDA}(L1_2)$
 $L1_2$
 A_3
 $L1_2$
 T_3
 H_{LDA}
 A_3
 $L1_2$

$(4^A)^{1/2}$

III. CONCLUSION

A

80.5 (A) A_3 D_{022} 84.0
 83.3 A_3 D_{023} 97.6 A_3 D_{022} 92.6
 53.8 A_3 49.7 A_3 D_{022} 55.6
 52.2 A_3 L_{12} f
 f 11

