[illegible]

[illegible],[1] [illegible],[1,*] [illegible],[2] and [illegible][1]

[1]N[illegible] R[illegible] E[illegible] L[illegible], G[illegible], C[illegible] 80201, USA

[2]U[illegible] E[illegible]-N[illegible], G[illegible]

(Received 24 [illegible] 2005; [illegible] 15 [illegible] 2006; [illegible] 13 [illegible] 2006)

[illegible] Al- [illegible] A) [illegible] Al [illegible] $L1_2$- [illegible] Al$_3$ [illegible] $L1_0$ [illegible] -T [illegible] Al$_3$ [illegible] $D0_{23}$ [illegible] Al$_2$ [illegible] 201) [illegible] $L1_2$ [illegible] $L1_0$ [illegible] Al$_3$ $L1_2$ [illegible] Al$_3$ [illegible] $D0_{23}$ [illegible] Al$_3$ [illegible] Al$_{13}$ [illegible] Al$_{14}$ [illegible] 4; [illegible] Al$_7$ [illegible] 5 [illegible] 301) [illegible] Al- [illegible].

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I. INTRODUCTION

[illegible][1,2] [illegible][3,4] [illegible][5–7] [illegible]

[illegible] $\mathcal{O}(10)$ [illegible] f.,
[illegible] 50 52) [illegible]

$$\Box H_{LDA}(\Box) \equiv E(\Box, V_{\Box}, \{R \quad x$$

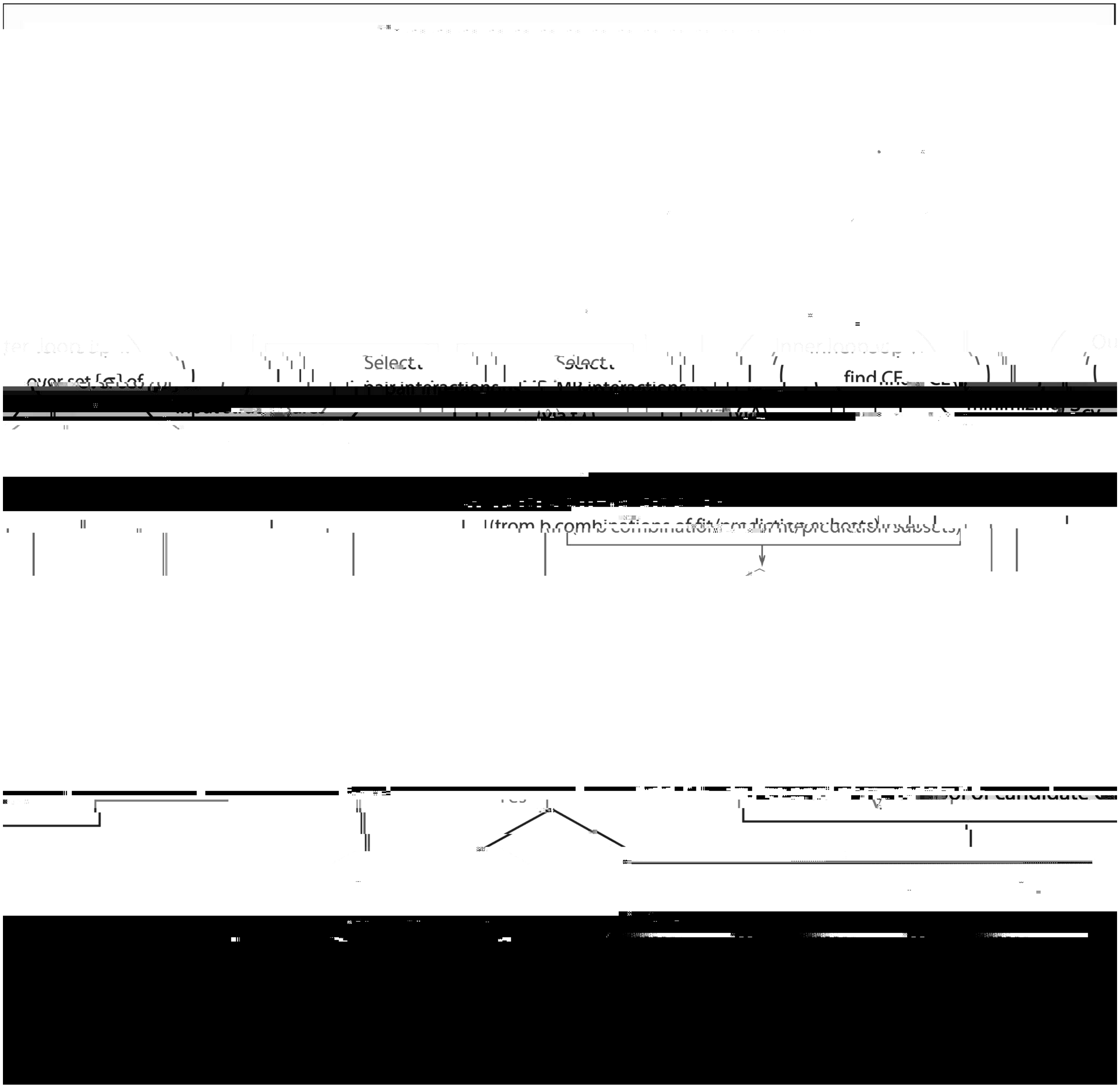
Select
Select
pair interactions
MB interactions
over set {σ} of
Inner loop
find CE
minimizing
(from b combinations of fit/prediction subsets)

FIG. 3. [illegible]

[illegible] 66 [illegible] 67. [illegible] $\{\Delta H_{LDA}(\sigma)\}$ [illegible] J [illegible],[61] [illegible].[61] [illegible] (5) [illegible]

$$D \ldots J \ldots (\ldots) = \ldots J(\ldots)|S(\ldots,\sigma)|^2, \quad (7)$$

[illegible] $S(\ldots,\sigma)$ [illegible]

$$\ldots_{MBCE} = \sum_{\sigma \notin \ldots} |\Delta H_{LDA}(\sigma) - \Delta H_{CE}(\sigma)|^2 + M, \quad (8)$$

$$M = \frac{1}{} J( )[\nabla^2]^{/2} J( ) = R D J^2 \qquad (9)$$

8) ... M ... J ... R, ... { , , } ...

... A).[62] ... [68 70] ... 100 ... 7 ...). ... N_{MB} ... A, ... 62. ... N ... 62) ... 1.)N ... S_{CV}) ... A ... N ... A ... [62] ... A ... 62 ... ~100 ...

... [66,67,71] ... A ... N_{MB} ... N_{MB} 2)$\cdots N_{MB}$ ... [72] ... N_{MB} ... N_{MB} ...

D. t t -st t s

... N(... A. ... 285 4 7 285 457 85 457 18.552 9 0 94 4 -524.4

[illegible] ΔH_{LDA} [illegible] $A_{1-x}B_x$ [illegible] ΔH_{CE} [illegible] ΔH_{CE} [illegible].

x	[illegible]	[illegible]	[illegible]	ΔH_{CE}	ΔH_{LDA}	[illegible] ΔH_{CE}
		[illegible] o 2				
1/9	A_8B	(301) A_8B	−45.1⋯−38.5		−39.4	−38.6
1/6	A_5B	(301) A_5B	−59.5⋯−55.9		−57.4	−57.3
1/5	A_4B	(201) [illegible] (301) A_4B	−71.3⋯−67.9		−67.3	−67.3
5/12	A_7B_5	(302) $A_2B_2A_3B_2A_2B$	−91.3⋯−89.1		−93.7	−93.7
		[illegible] o 3				
1/5	$A_{12}B_3$	(301) A_5BABA_6B	−71.0⋯−67.9		−67.5	−68.5
4/15	$A_{11}B_4$	(401) A_5BABA_4BAB (2 [illegible], [illegible] f. 14)	−86.6⋯−84.9		−85.4	−85.7
2/5	A_9B_6	(401) $A_4B_4A_4BAB$	−92.9⋯−91.6		−93.6	−89.5
2/3	A_4B_8	(302) $B_5A_2B_3A_2$	−69.0⋯−63.2		−58.7	−62.4
	A_2B_4	(301) A_2B_4	−68.6⋯−66.4		−59.1	−58.4
		[illegible] o 4				
2/11	A_9B_2	(301) A_5BA_4B	−64.9⋯−62.3		−62.5	−63.9
1/3	$A_{10}B_5$	(401) $A_4BABA_2BA_2BAB$	−91.9⋯−87.8		−87.8	−87.9
	A_8B_4 ([illegible].4905)	(302) $A_5B_2A_3B_2$	−95.7⋯−85.4		−91.1	−88.2
2/5	A_3B_2	(110) A_2BAB	−94.0⋯−86.7		−89.4	−89.8
5/8	A_3B_5	(401) B_4A_2BA	−75.6⋯−68.2		−64.1	−66.6
2/3	A_4B_8	(601) B_6ABA_2BA	−68.2⋯−61.6		−60.7	−59.7
		[illegible] o 5				
1/6	$A_{10}B_2$	[illegible]	−62.2⋯−54.2		−55.3	−55.3
1/5	A_8B_2	[illegible]	−71.5⋯−66.5		−66.5	−67.4
1/3	A_8B_4 ([illegible].4557)	$A_3BA_2BA_3B_2$ (201)	−91.2⋯−88.8		−91.1	−90.4
7/12	A_5B_7	(302) $B_2A_2B_3A_2B_2A$	−94.4⋯−91.9		−74.8	−77.2
		[illegible] o 6				
1/9	$A_{18}B_2$	[illegible]	−37.9⋯−34.8		−34.4	−35.0
2/17	$A_{15}B_2$	(401) $A_{14}BAB$	−43.0⋯−41.4		−41.0	−41.3
4/17	$A_{13}B_4$	(401) A_6BABA_5BAB (2 [illegible], [illegible] f. 14)	−81.5⋯−78.9		−79.9	−80.4
1/2	A_3B_3 ([illegible].55)	(111) A_3B_3	−41.3⋯−7.4		−11.6	−11.7
		[illegible] o 7				
1/11	$A_{10}B$	(301) $A_{10}B_1$	−32.7⋯−31.7		−31.4	−32.2
2/13	$A_{11}B_2$	(301) A_6BA_5B	−54.7⋯−53.2		−53.3	−54.6

[illegible]E AND RANGE OF INTERACTIONS REQUIRED FOR DESCRIBING L[illegible]

[illegible] $L1_2$ [illegible] $D0_{23}$) [illegible]

[illegible] $L1_2$) [illegible] ⋯, [illegible] (α=$L1_2$, $D0_{22}$, $D0_{23}$) [illegible] 12 [illegible] 2 [illegible]):

[illegible] A [illegible] B [illegible] A_3B [illegible] AB_3 $L1_2$). [illegible]

[illegible] A_3B [illegible] AB_3 [illegible].

[illegible] $L1_2$, $D0_{22}$ [illegible] $D0_{23}$ [illegible]

[illegible] $D0$

[illegible] $(^{1)} = 10$ [illegible] $(^{7)} = 8$. [illegible]

[illegible] [[illegible] . 8 (

1. Ground-state search at different outer-loop iterations

f. 10 … o (=1 … =7). … 16 (=1) … 20 (=7)

f. 4,

f. 9). … =1,

A … 10)] … ΔH_{CE} … ΔH_{LDA} … =0 … A.

f. 3) … 40% 96 -49

x				ΔH_{CE}	ΔH_{LDA}

FIG. 10. [illegible] ($=1$) [illegible] ($=7$ [illegible]). All [illegible]

[illegible] $=1$.

2. Illustrating the outer-loop history

[illegible] 11 [illegible] A), [illegible] $L1_2$-[illegible] ($L1_2/D0_{22}/D0_{23}$) [illegible] 11, [illegible]

[illegible] $=1$ [illegible] 11 [illegible] $=1$ [illegible] $=1$.

[illegible] CE [illegible] LDA [illegible]

[illegible] CE [illegible] LDA [illegible] $L1_2$-[illegible] $=1$ [illegible]

[illegible] [301) A_8B], [illegible] [301) A_5B], [illegible] [301) A_4B] [illegible]

[illegible] $=1$ [illegible] 11 [illegible]

[illegible] $L1_2$-[illegible] $L1_2$-[illegible]

[illegible]	[illegible]	$N=28$ [illegible] $=1$	$N=32$ [illegible] $=2$	$N=37$ [illegible] $=3$	$N=43$ [illegible] $=4$	$N=47$ [illegible] $=5$	$N=51$ [illegible] $=6$	$N=53$ [illegible] $=7$
[illegible]	[illegible] ($D0_{23}$)	0%	88%	92%	62%	64%	100%	100%
[illegible]	[illegible] $L1_2/D0_{22}/D0_{23}$ [illegible]	0%	88%	92%	62%	64%	100%	100%
[illegible]	[illegible] ($L1_2$)	40%	100%	100%	92%	79%	100%	100%
[illegible]	[illegible] $L1_2/D0_{22}/D0_{23}$ [illegible]	0%	37%	100%	85%	79%	100%	100%

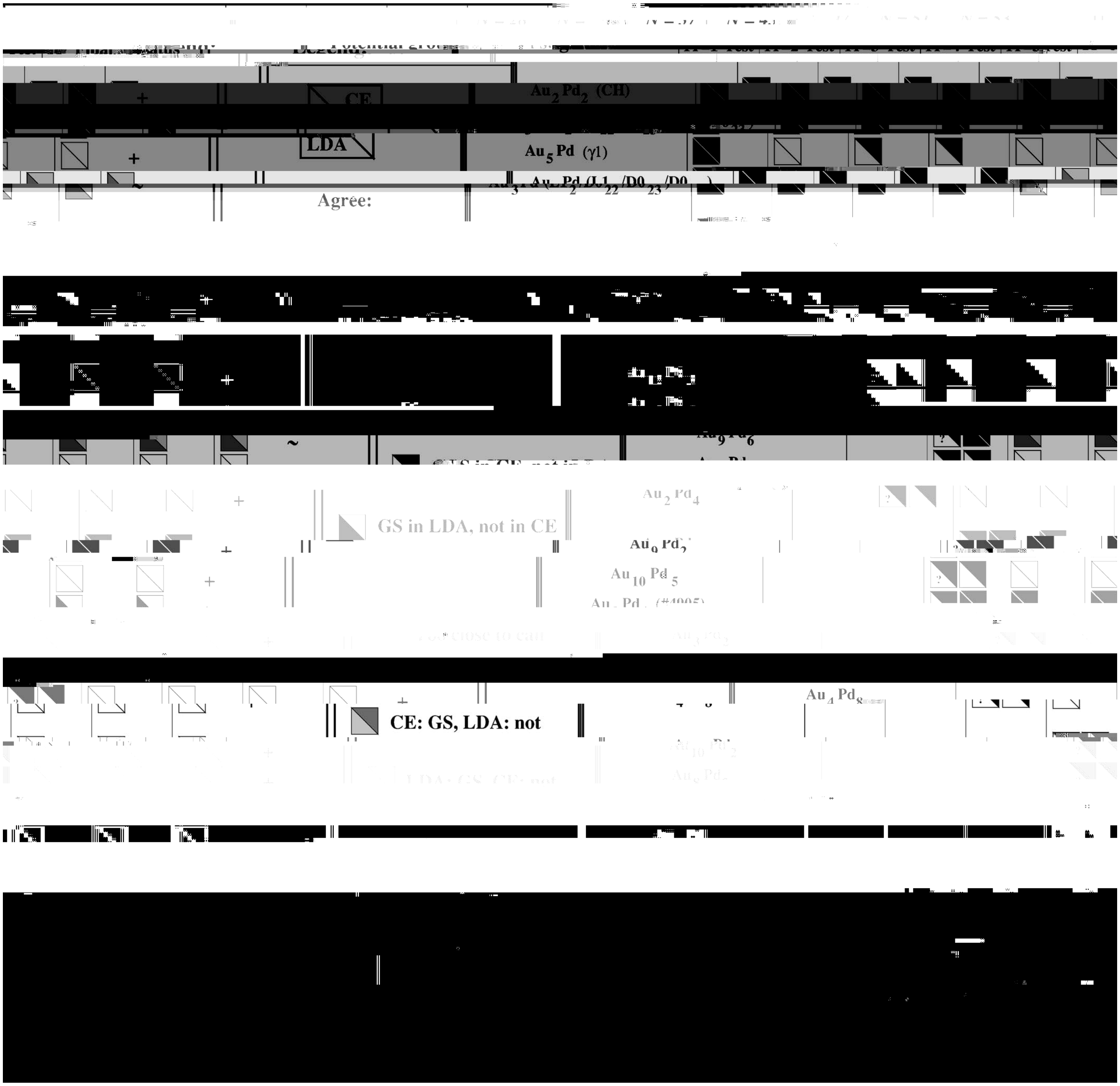

FIG. 11. [illegible]

[illegible] f.

[illegible]) *CE* [illegible] *LDA* [illegible] A [illegible] Au$_8$ [illegible], Au$_5$ [illegible] Au$_7$ [illegible] 5.

[illegible]) *CE* [illegible] *LDA* [illegible] A [illegible] Au$_4$ [illegible].

[illegible]) *S* [illegible] *LDA* [illegible] *x* [illegible].[85] [illegible] H_{LDA} [illegible] Au$_7$ [illegible] 5, [illegible] Au$_2$ [illegible] 1) [illegible] A [illegible].

3. Generic behaviors during outer-loop iterations

[illegible] f. 11, [illegible].

[illegible]) A [illegible] Au [illegible] 3 $L1_2$.

[illegible]) A [illegible] A [illegible]

, S_{CV} … x … $\{\Delta H_{LDA}\}$ …

… 37 … ΔH_{LDA} …

ΔH_{CE} … 13. … 2.8 …

II. DI C7 I ON OF GR 7 ND- A E ORDERED- R7 C 7 RE IN A $_{1-x}$ $_x$

… A … 14. …

A. … A $_{1-x}$ $_x$ m s, x 0.22: (301) " t st t s

… [87] … [87] … (301) … (301) … 14. … 87, … E_{CS} … 2) … 12) … E_{CS} … ΔH_{LDA} … $_{1-x}$ $_x$ … 12) … (001) …

… f . 12)],

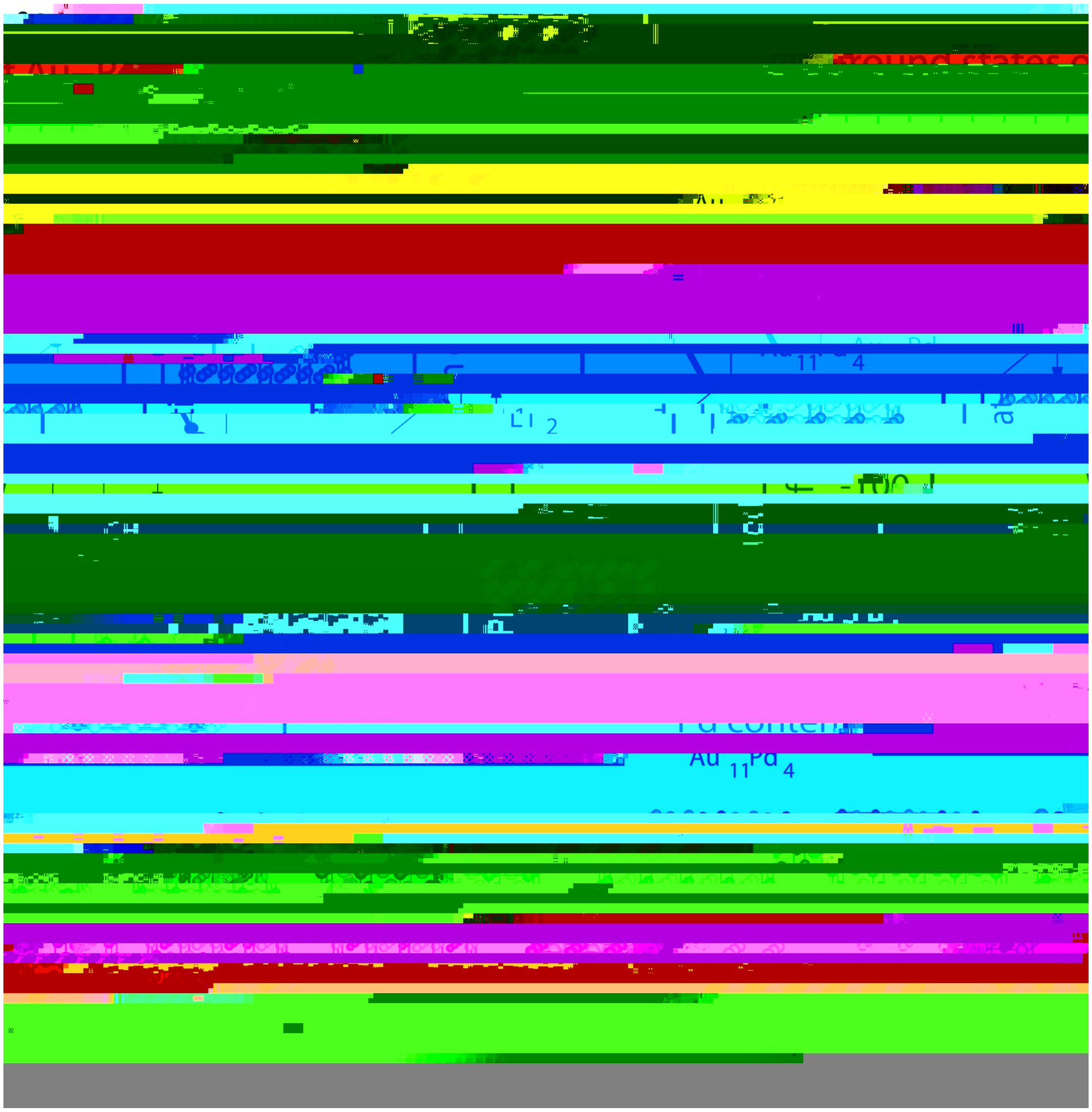

FIG. 14. [illegible]

[illegible]

E. [illegible]

[illegible]

[illegible] N_0 [illegible] N_0 [illegible] 15 [illegible] $N_0 = 176$ [illegible] 3×10^6 [illegible]

[illegible] $x = 1/3$, [illegible] $C37$, [illegible] 15 [illegible] [77,92] [illegible] ~10 [illegible] $L1_1$, [illegible] 15 [illegible] $E = 5.463$ [illegible] $E = 5.475$ [illegible] $L1_2$. [illegible] $x = 1/3$. [illegible] H_{LDA} [illegible] H_{LDA} ($C37$). [illegible] $C37$ [illegible] $C37$ [illegible] 15 [illegible]

[illegible] [15] [illegible] $D0_{23}$ [illegible] 15, [illegible] H_{LDA} ($L1_2$) [illegible] 12 [illegible] $L1_2$ [illegible] 15 [illegible] $L1_2$ [illegible] T [illegible] $L1_2$ [illegible] H_{LDA} [illegible] $L1_2$ [illegible] 15.

III. C[illegible]

[illegible]

[illegible] 6004 [illegible]

80.8 (A) 80.5 A Al$_3$ $D0_{22}$ 84.0 83.3 Al$_3$ $D0_{23}$, 97.6 92.6 Al 53.8 49.7 Al$_3$ $D0_{22}$ 55.6 52.2 Al$_3$ $L1_2$. [11]

[78] [illegible], [illegible] 2 [illegible] + [illegible], [illegible], [illegible], 2001.

[79] [illegible] A. **30**, 244 [illegible] 1944).

[80] [illegible]

[81] [illegible] 1), [illegible] 3 [illegible] $D0_{23}$ [illegible] $L1_2$ [illegible] $D0_{22}$. [illegible] $D0_{23}$ [illegible] $L1_2$ 123