Chapter 14
Atomistic Pseudopotential Theory of Droplet Epitaxial GaAs/AlGaAs Quantum Dots

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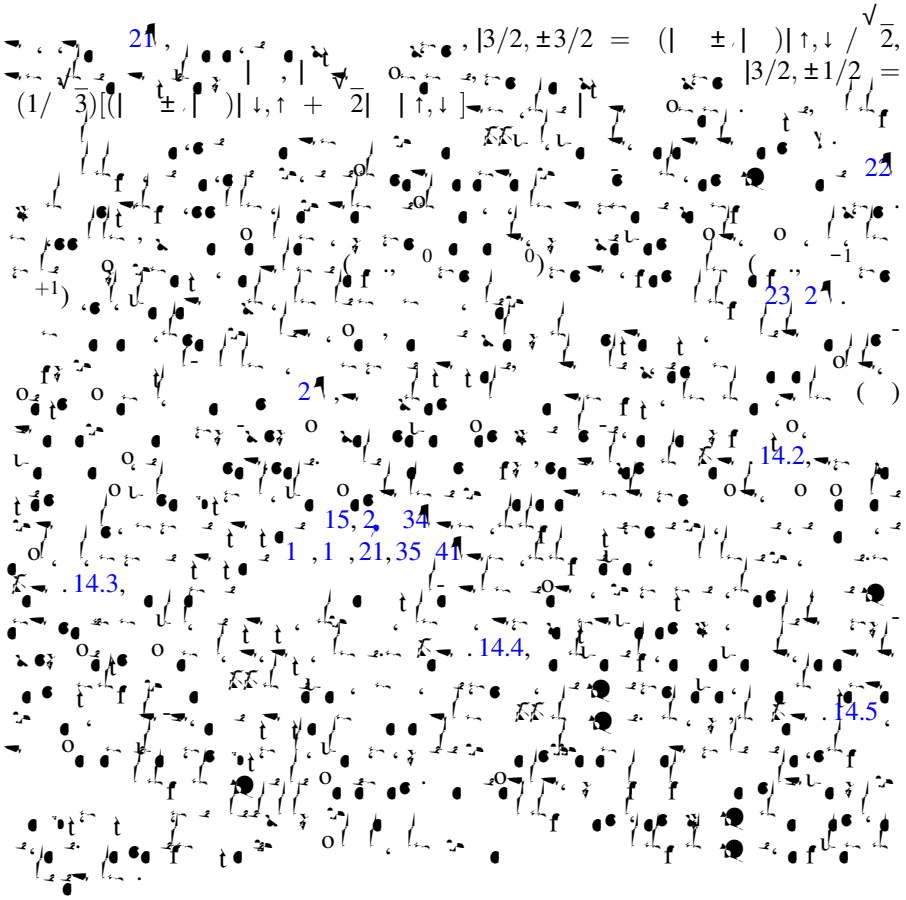
Abstract



14.2 Atomistic Many-Body Pseudopotential MPseual00.20510004svoffm39

[illegible] 2 ,42 4 [illegible]

[illegible] 45, 46, 4 [illegible]

$$= \sum\sum \frac{3}{} \left[\alpha^{(1)}\Delta \;{}^{2} + \alpha^{(2)}\Delta \;{}^{3}\right]$$

$$+ \sum\sum_{<} \frac{3\beta}{{}^{0}\;{}^{0}} \left[(\mathbf{R_j} - \mathbf{R_i}) \cdot (\mathbf{R_k} - \mathbf{R_i}) - \theta^{0}\;{}^{0}\;{}^{0}\right]$$

$$+ \sum\sum_{<} \frac{3\sigma}{\sqrt{{}^{0}\;{}^{0}}} \Delta \left[(\mathbf{R_j} - \mathbf{R_i}) \cdot (\mathbf{R_k} - \mathbf{R_i}) - \theta^{0}\;{}^{0}\;{}^{0}\right], \quad (14.1)$$

$\Delta \;{}_{} = \left[(\mathbf{R_i} - \mathbf{R_j})^2 - ({}^{0})^2\right] / {}^{0}$, $\mathbf{R_i}$ [illegible] θ^{0} [illegible] $= 4$ [illegible] $\alpha^{(1)} (\equiv \alpha), \beta$ [illegible] σ [illegible] 46

$${}_{11} + 2 \;{}_{12} = \sqrt{\frac{3}{4\;{}^{0}}}(3\alpha + \beta - 6\sigma)$$

$${}_{11} - \;{}_{12} = \sqrt{\frac{3}{{}^{0}}}\beta$$

$${}_{44} = \sqrt{\frac{3}{{}^{0}}}\frac{\alpha\beta - \sigma^2}{}$$

Fig. 14.1

$$(\mathbf{R_{12}}, \mathbf{R_{23}}, \mathbf{R_{34}}) = (1+\varepsilon) \cdot (\mathbf{R^0_{12}}, \mathbf{R^0_{23}}, \mathbf{R^0_{34}}). \tag{14.3}$$

35, 46, 4

anostru.3F2 1 Tf 1.99740004 0 TD 0 Tc (1)Tj372911413430344779

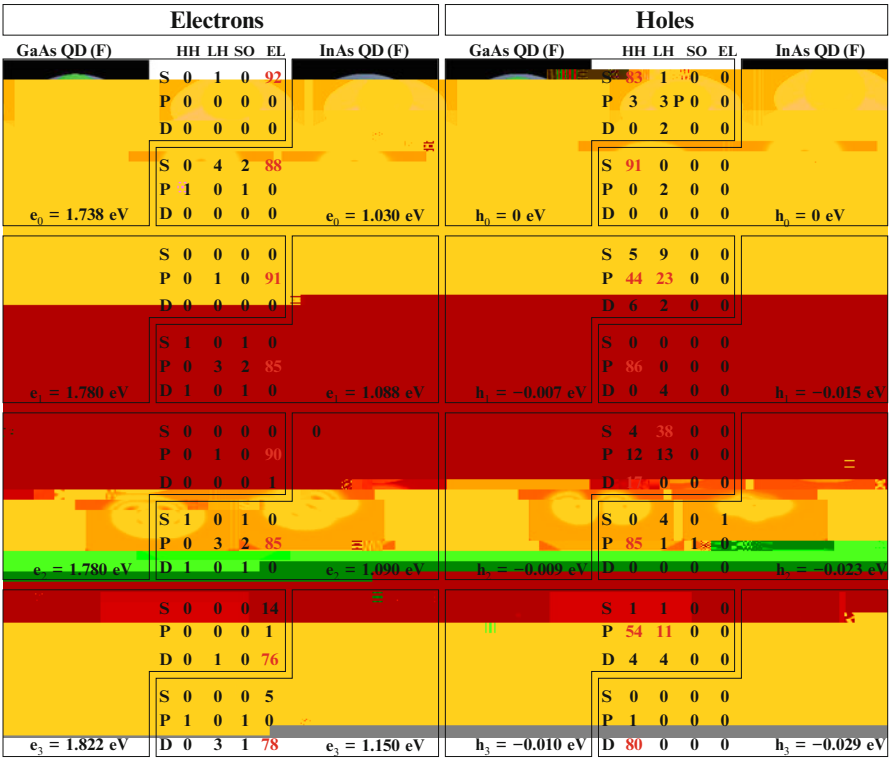
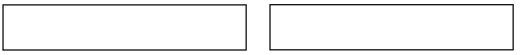
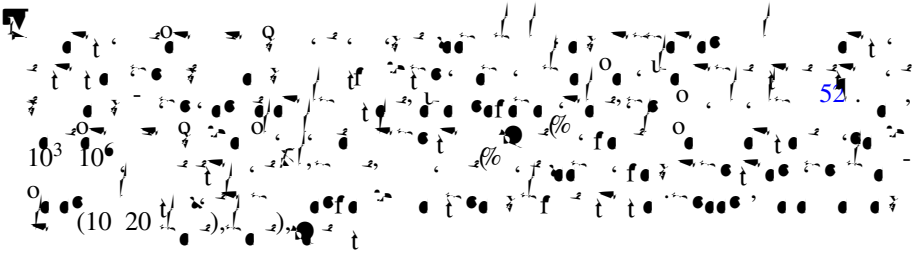

Electrons
Holes
GaAs QD (F)
HH LH SO EL
InAs QD (F)
S 0 1 0 92
P 0 0 0 0
D 0 0 0 0
S 0 4 2 88
P 1 0 1 0
D 0 0 0 0
e0 = 1.738 eV
e0 = 1.030 eV
S 83 1 0 0
P 3 3 P 0 0
D 0 2 0 0
S 91 0 0 0
P 0 2 0 0
D 0 0 0 0
h0 = 0 eV
h0 = 0 eV
S 0 0 0 0
P 0 1 0 91
D 0 0 0 0
S 1 0 1 0
P 0 3 2 85
D 1 0 1 0
e1 = 1.780 eV
e1 = 1.088 eV
S 5 9 0 0
P 44 23 0 0
D 6 2 0 0
S 0 0 0 0
P 86 0 0 0
D 0 4 0 0
h1 = −0.007 eV
h1 = −0.015 eV
S 0 0 0 0
P 0 1 0 90
D 0 0 0 1
S 1 0 1 0
P 0 3 2 85
D 1 0 1 0
e2 = 1.780 eV
e2 = 1.090 eV
S 4 38 0 0
P 12 13 0 0
S 0 4 0 1
P 85 1 1 0
D 0 0 0 0
h2 = −0.009 eV
h2 = −0.023 eV
S 0 0 0 14
P 0 0 0 1
D 0 1 0 76
S 0 0 0 5
P 1 0 1 0
D 0 3 1 78
e3 = 1.822 eV
e3 = 1.150 eV
S 1 1 0 0
P 54 11 0 0
D 4 4 0 0
S 0 0 0 0
P 1 0 0 0
D 80 0 0 0
h3 = −0.010 eV
h3 = −0.029 eV

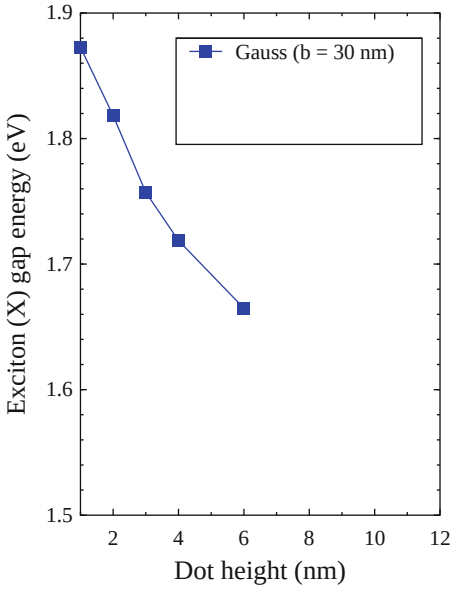
Fig. 14.2



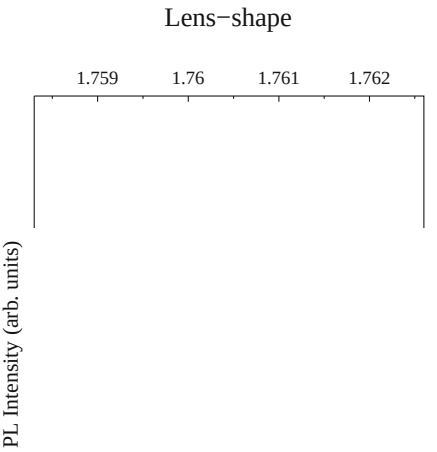
-0.5 -

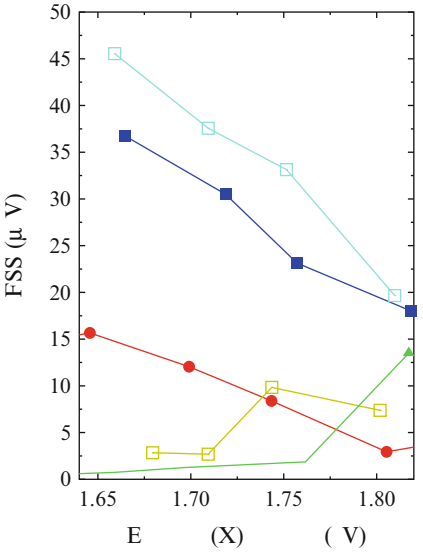
14.3 Geometry of Epitaxial GaAs/(Al,Ga)As QDs as Seen by Excitonic Spectroscopy




Gauss (b = 30 nm)
Exciton (X) gap energy (eV)
Dot height (nm)
1.9
1.8
1.7
1.6
1.5
2
4
6
8
10
12

[illegible] 1 [illegible] 14 [illegible] 5 , 62 , [illegible] 25, 56, 60, 63, 64 [illegible] 14 [illegible] (001)- [illegible] 5 [illegible] 2.3 ± 0.6 [illegible] (311) - [illegible]


Lens−shape
1.759
1.76
1.761
1.762
PL Intensity (arb. units)


50
45
40
35
30
25
20
15
10
5
0
FSS (μ V)
1.65
1.70
1.75
1.80
E (X) (V)

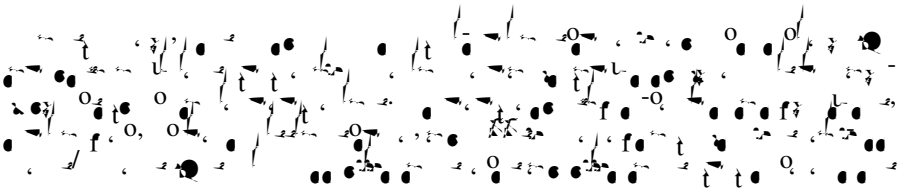


Table 14.1

			(%)	
00	0. 0.2	10, .5, 2.5	0	0
01		45, 45, 3	35	35
02		0, 50, 3	45	45
03		0, 50, 3	35	45
04		60, 40, 2	35	45
05		25, 31, 3	35	35
06		30, 30, 3	30	30
0		30, 30, 4	30	30
0		30, 30, 6	30	30
0		35, 30, 3	30	30
10		35, 30, 4	30	30
11		35, 30, 6	30	30
12	0.06 0, 4	30, 30, 3	30	30
13	0.06 0, 4	30, 30, 6	30	30
14	0.06 0, 4	35, 30, 3	30	30
15	0.06 0, 4	35, 30, 6	30	30

110 110

21 . (2012)

14.1. 46 43, 46 .14.2. 4 .14.2 12 12),

$$= {}_2 + \delta \quad {}_1 + \quad , \tag{14.14}$$

2 2 δ 1·

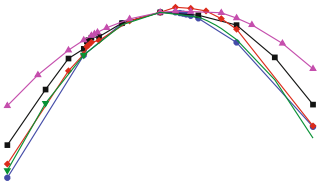
|1 |2

$$= \begin{pmatrix} {}_1 + \delta\ {}_1 + \gamma_1 & \varepsilon_0/2 \\ \varepsilon_0/2 & {}_2 + \delta\ {}_2 + \gamma_2 \end{pmatrix}. \tag{14.15}$$

Table 14.2

00	1363	>	0.15	+ 2 3
01	1644	0.1	0.11	+1
02	1650	0.1	0.0	−4
03	1643	0.1	0.0	−4
04	1 42	0,	0.14	−43
05	16 ,	0.3	0.33	+2,
06	1 62 ± 2	0. ± 0.3	0. 5 ± 0.0	−21 ± 5
0	1 1 ± 2	0.4 ± 0.1	0, 5 ± 0.06	−26 ± 3
0	1666 ± 1	0, ± 0.	1.06 ± 0.0	−25 ± 2
0,	1 54	0,	0. ,	−33.5
10	1 14	0.4	0.	−3 .4
11	1660	0.	0, 6	−40.5
12	1 06 ± 5	1.2 ± 0.	0. 4 ± 0.11	−14 ±
13	1 2 ± 2	1.2 ± 0.5	0. 5 ± 0.0,	−15 ±,
14	1 ,, ± 2	1.3 ± 1.0	0. 3 ± 0.03	−25 ± 6
15	1 21 ± 2	1. ± 1.4	0. 4 ± 0.0	−40 ± 5

21



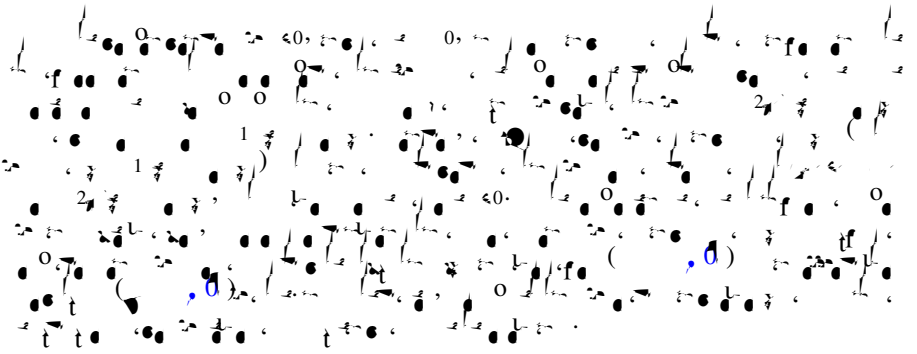
(14.15)), (δ 1).

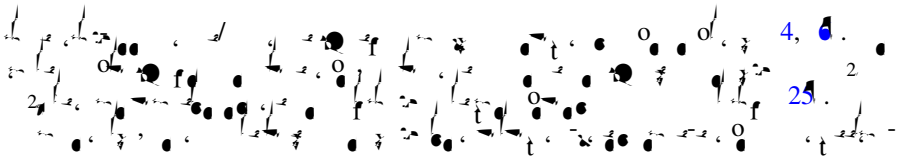
γ γ (14,) (14.). 1 2 oo γ γ (01, 02, 03, 04, 05 3.5%, 2.4%, 2.6%, 5.0%, .2%,) 14. 10%, −100 +100 .

0 0 0 0 (14.1) (14.1,) (= 0)

$$_0 = \frac{\Delta \quad 2\theta}{\gamma} \qquad _0 = -\Delta \quad 2\theta, \tag{14.20}$$

Δ = 0. 0 γ θ (14.20). 14.2 00. Δ θ is large,





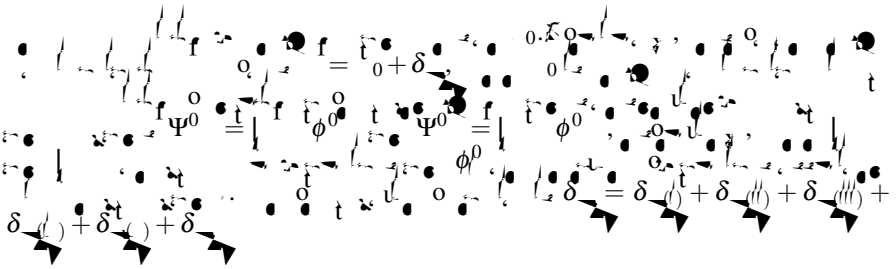
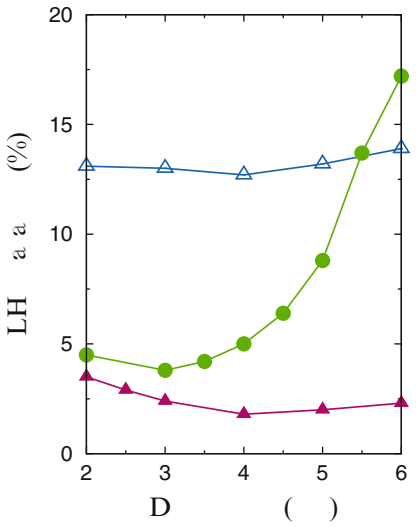
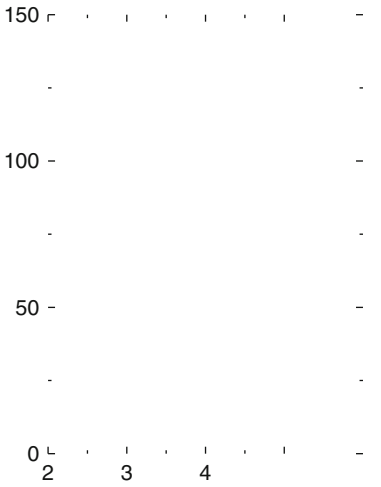
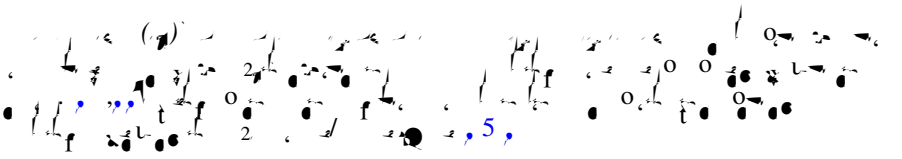


Table 14.3 ... 0, 1, 2 ... 0.6, 0.4 ...

...	/ (%)		
...	(0)	(1)	(2)


20
15
10
5
0
2
3
4
5
6
(%)
D
( )


150
100
50
0
2
3
4



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