Localized in erface t a e in coheren i ovalen emiconduc or he erojunc ion

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1,2,* A 3,†

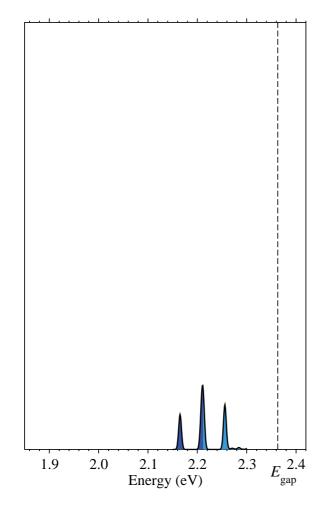
D a a REMRSEC, C a S M , G , C a 80401, USA

2Na a R a E La a , G , C a 80401, USA

3U C a , B , C a 80302, USA

13 A 2011; 16 S 2011; 22 G 201
        ^{1}P
                                                                                                              2011)
    (
                            V
417252()- (15456.5 0004172.-.5())-735.4(- - ()-.5(4())-0496.(B)) s)-3-0494-456.5()-5607
                                                                                                                                               4172486
```





B. Compu ing the QW eigen t a e

 $\begin{bmatrix}
-\frac{1}{2}\nabla^{2} + \sum_{n} \widehat{v} (\vec{r} - \vec{R}_{n}, \underline{n}) + \widehat{V} \\
v (\vec{r} - \vec{R}_{n}, \underline{n})
\end{bmatrix} | i \rangle = E_{i} | i \rangle, \quad (3)$

$$\vec{R}_n$$
:
$$v(\vec{r},) = v(\vec{r},0) + \mathbf{T}(), \qquad (4)$$

T
$$\hat{V}$$

T $V(\vec{r},0)$
 $V(\vec{r},0)$

ŧ.

M

(3)

C. L $\mathbf{q_t}$ ice relax \mathbf{q} ion by \mathbf{t} rain minimiz \mathbf{q} ion

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В,

A. Model of in erface tae in a ingle he erojunc ion

1930 , T ²⁶ S . T

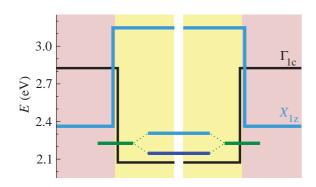
.

J 28 ,

, T T ,²⁹

A B. I S_{A} - , , CB V^{B} , 7.8 () , () , , (X.T , () X.T , ()

B. Appearance of a $% \left(1\right) =\left(1\right) =\left(1\right)$ in B. Appearance of a $% \left(1\right) =\left(1\right$



- . (7)

F CA F B 84, 125315 (2011)

		a_{SO}		a	b	C
			, c	A , : 5.6533 A	A	
;	131.8	5.1346 - 09	0.4558	-2.04999109+00	$1.715\ 650\ 28\ +00$	$0.000\ 000\ 00\ +00$
				7.16475874-02	$2.946\ 307\ 27\ -02$	$7.354\ 110\ 60\ -09$
				$3.856\ 523\ 14\ -06$	$2.901\ 070\ 82\ -05$	$2.824\ 113\ 28\ -05$
				$-4.430\ 377\ 80\ -06$	4.525 175 88 +04	1.062 455 06 +00
A	75.0	1.4621 - 01	0.0000	-7.25809634-01	$1.278\ 931\ 35\ +00$	$0.000\ 000\ 00\ +00$
				$1.711\ 100\ 80\ -08$	2.480 896 24 +01	9.72784996-05
				$2.339\ 343\ 68\ -01$	1.891 093 76 +00	$1.518\ 192\ 74\ +00$
				-1.04139817+00	$1.379\ 048\ 51\ +00$	$4.882\ 919\ 62\ -01$
				, : 5.8687 A		
	131.8	2.1419 - 11	0.5250	$-1.637\ 360\ 60\ +00$	1.46988647+00	$0.000\ 000\ 00\ +00$
				$2.080\ 145\ 97\ -01$	1.773 726 03 +01	1.684 469 70 +00