Electronic-Structure Theory of Semiconductor Quantum Dots

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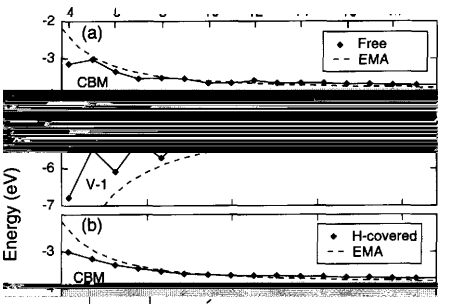
The "Standard Model" of the Electronic Structure of Dots

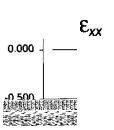
Progress made in the growth of "free-standing" (e.g., colloidal) quantum

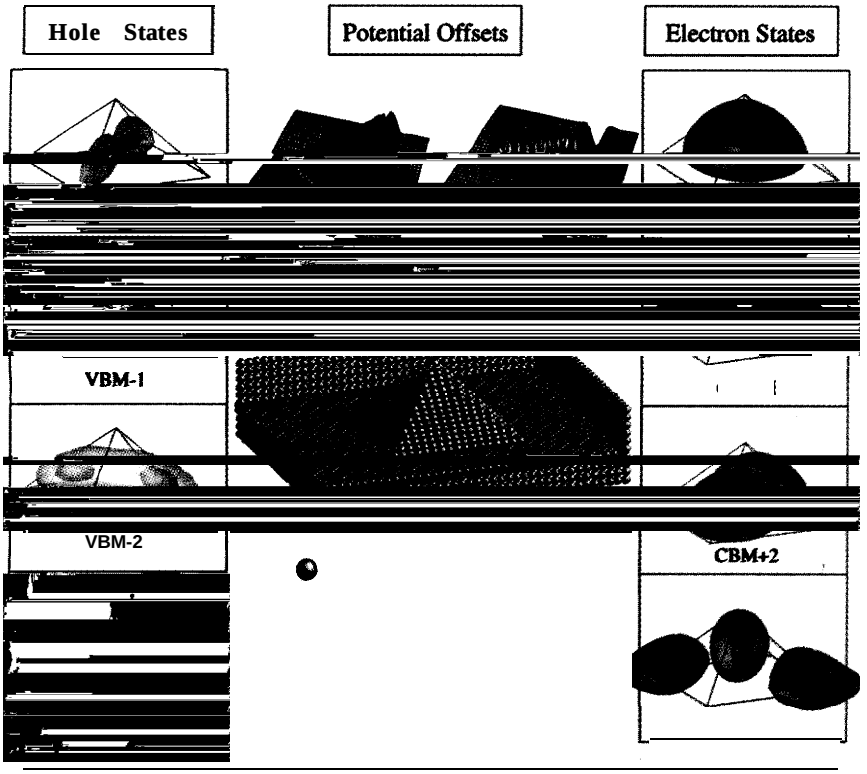


GaAs)

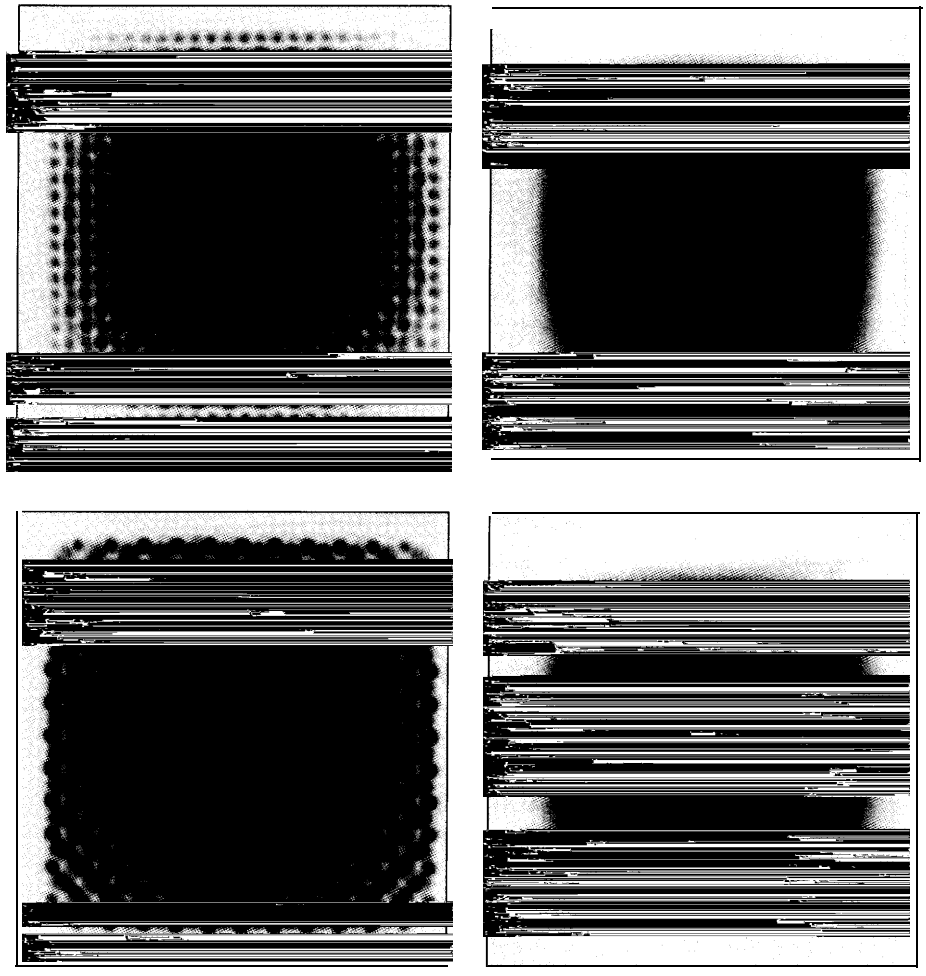
field.[20]

$$\rho_{\mathbf{q}}(\mathbf{r}) = \sum_{\mathbf{G}} \rho_{\mathbf{G}}(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}}$$




Hole States
Potential Offsets
Electron States
VBM-1
VBM-2
CBM+2

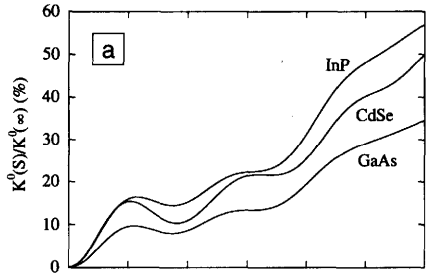
wave functions, transition probabilities, etc. On a massively parallel CRAY

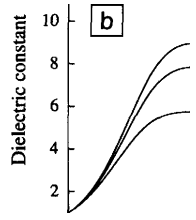


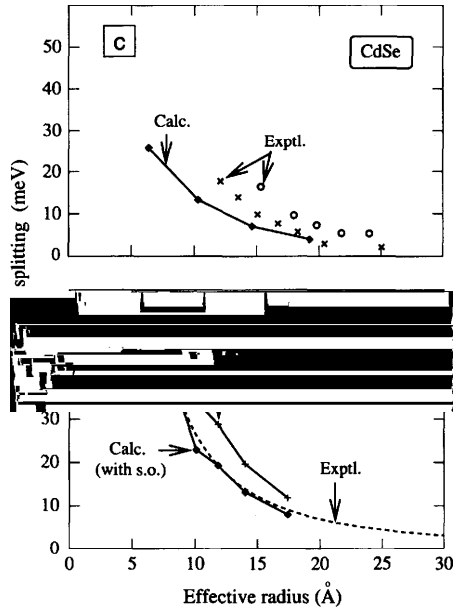
$$\langle \Phi_{ij} | \mathcal{H} | \Phi_{kl} \rangle = (\varepsilon_{j,c} - \varepsilon_{i,v})\delta_{i,k}\delta_{j,l} - J_{ij,kl} - K_{ij,kl} \quad (5)$$

$$\int\int \frac{\psi^*_{i,v}(\mathbf{x}_1)\psi^*_{j,c}(\mathbf{x}_2)\psi_{k,v}(\mathbf{x}_1)\psi_{j,c}(\mathbf{x}_2)}{\bar{\varepsilon}(\mathbf{r}_1,\mathbf{r}_2)\,|\mathbf{r}_1-\mathbf{r}_2|}\,d\mathbf{x}_1 d\mathbf{x}_2$$

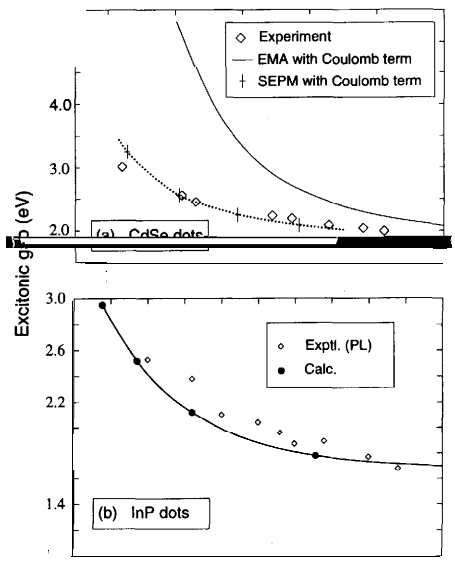
$$\int\int \frac{\psi^*_{i,v}(\mathbf{x}_1)\psi^*_{j,c}(\mathbf{x}_2)\psi_{j,c}(\mathbf{x}_1)\psi_{k,v}(\mathbf{x}_2)}{\bar{\varepsilon}(\mathbf{r}_1,\mathbf{r}_2)\,|\mathbf{r}_1-\mathbf{r}_2|}\,d\mathbf{x}_1 d\mathbf{x}_2 .$$

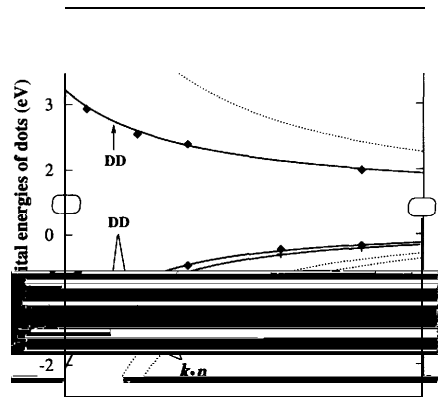


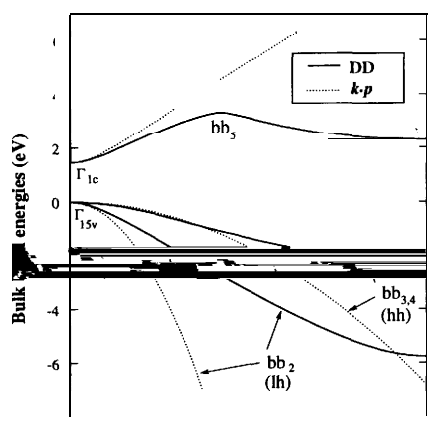




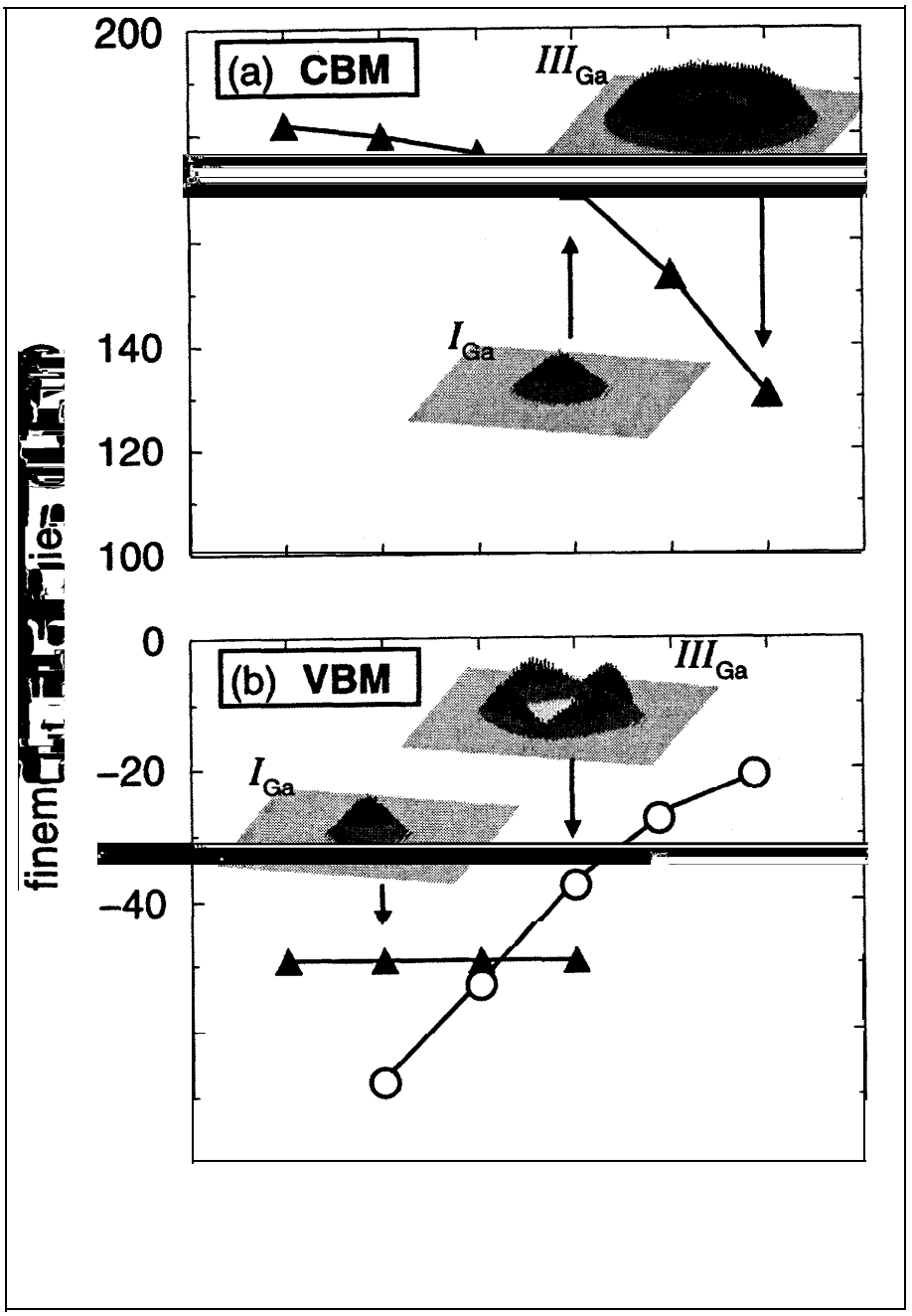
$$\left(\frac{a_x}{R}\right)^3 E_x$$


Experiment
EMA with Coulomb term
SEPM with Coulomb term
4.0
3.0
2.0
(a) CdSe dots
Excitonic gap (eV)
3.0
2.6
2.2
1.4
Exptl. (PL)
Calc.
(b) InP dots


3
2
0
-2
DD
DD
k·p


DD
k·p
2
0
-4
-6
hh3
Γ1c
Γ15v
bb3,4
(hh)
bb2
(lh)

gies versus size is consistently too large
in k · **p.**
A recent


200
140
120
100
0
−20
−40
(a) CBM
(b) VBM
III_Ga
I_Ga
III_Ga
I_Ga