1. : A B A

single-particle electronic

(A)

1 3 A

(k = 0) A

1 6 free-standing fit

A accommo-

date predicts . semiconductor-embedded ,

A / A , 26 .

(A) 7 , (,

) ~10^3 10 ( )

A A

many-body description

( ) (10^3 10)

A 8 ,

( ) 9

multi-band coupling (A),

arbitrary shapes and materials, realistic surface

(multiplet) 10^3 10^5 atoms ( ).

2. [illegible]

2.1 [illegible]

1. The shape, size and composition of the dot are accepted as "input", [illegible]

2. Atoms are relaxed to their strain-minimizing positions [illegible] C_{11}, C_{12}, C_{44} [illegible]

3. The single-particle screened pseudopotential is fit to bulk solids: [illegible] $R_{n\alpha}$ [illegible]

$$V_{\text{[illegible]}} + V_{\text{[illegible]}} = \sum_{n,\alpha} V_\alpha(r - R_{n,\alpha}) . \quad (1)$$

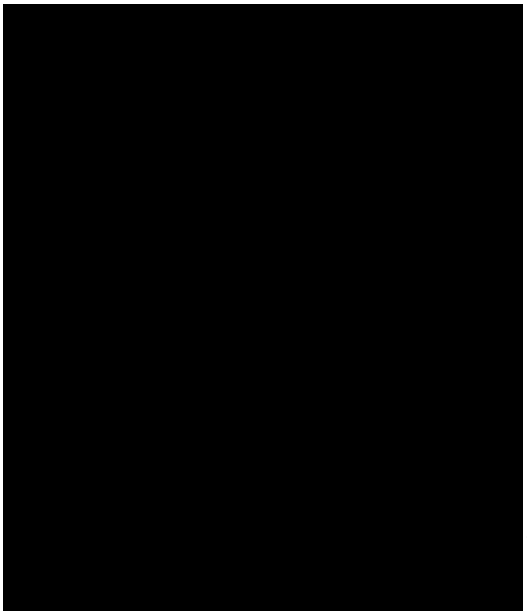
[illegible] V_α [illegible]

4. The wavefunctions are expanded in plane-waves, [illegible]

5. The pseudopotential-plane wave Hamiltonian is diagonalized incredibly rapidly [illegible] 10000 [illegible] 20000 [illegible] 19999 [illegible] (= [illegible] 20000) [illegible] (= 20001). [illegible] $\approx$19999 [illegible] $(H - A)^2$. [illegible]

2.2. B: T e a -b d b e

1. Inter-electronic integrals are computed numerically:



3. Established an energy-level model for the "semiconductor embedded" self-assembled InAs/GaAs dots 23 29 .

3.2 T e a acc e -da ef e e ed a e-e e b e

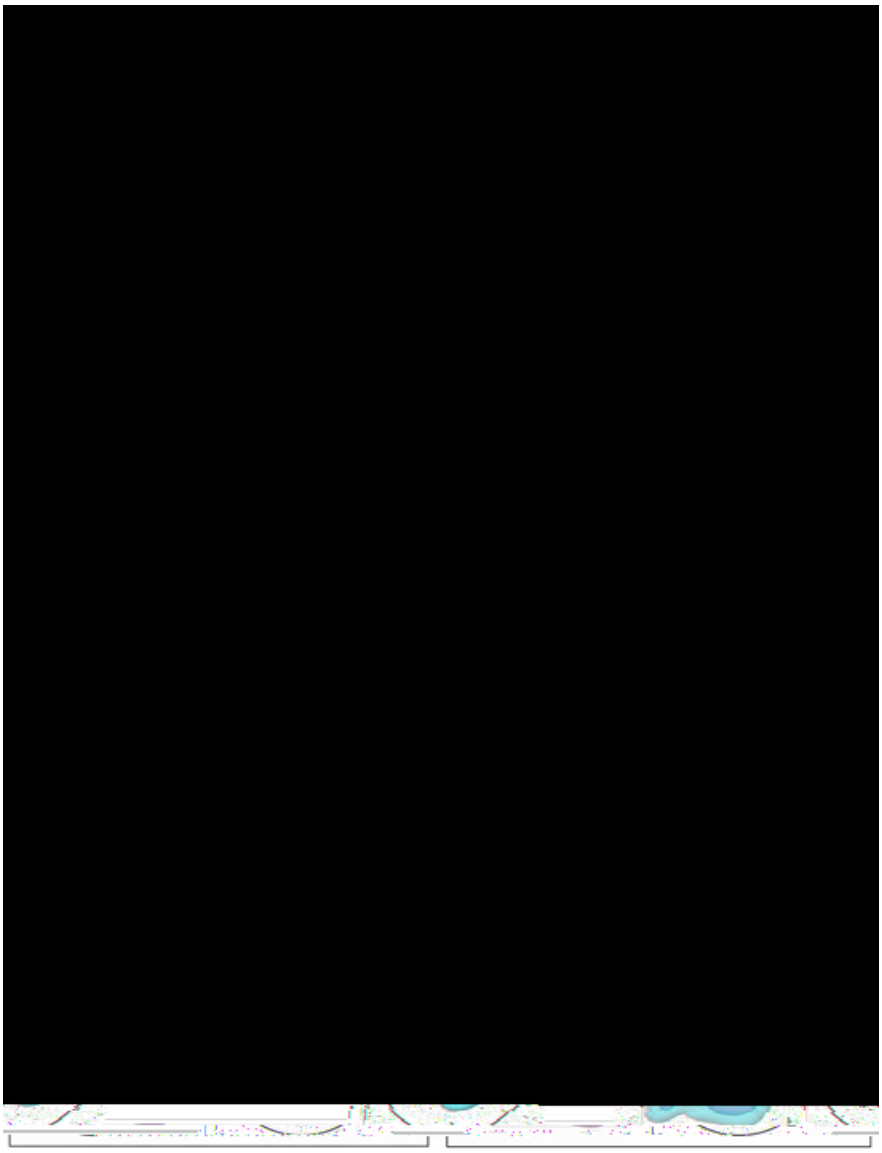
1. Predicted the electron-addition energies in freestanding InAs 30, 31 and CdSe 32 dots,

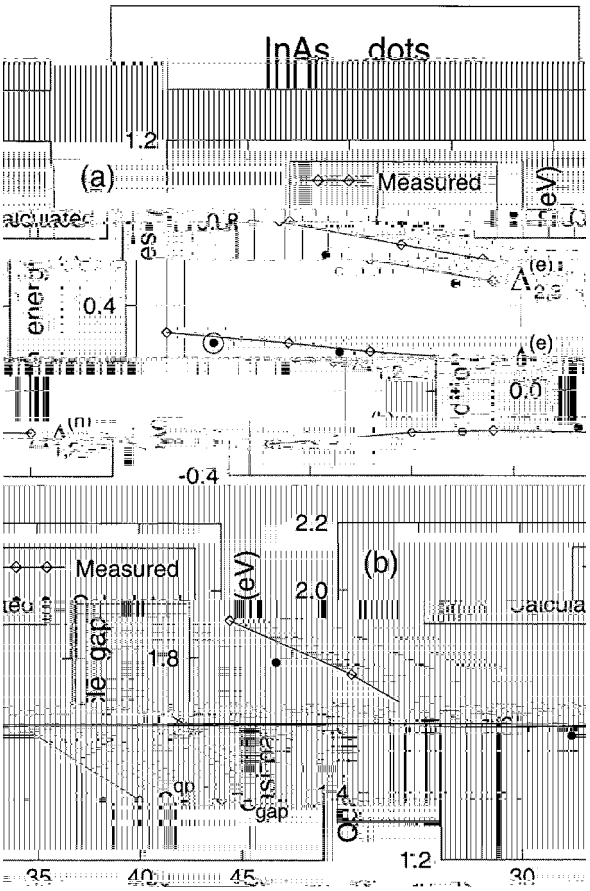
2. Established deviations from Hund's rule as well as "spin-blockade" 32 .

3.3 T e a acc e -da e, f e v-e e b e

Established theory of electron hole exchange in dots , 9, 17 .

$\Delta_x \sim \bar{R}^{-3}$.




InAs dots
(a)
Measured
1.2
0.8
0.4
0.0
-0.4
(eV)
2.2
2.0
(b)
Measured
1:8
1:2
35
40
45
30
Dot diameter (Å)

4.

H. FU, A. ZUNGER, . . . 57, 1 064 (1998).
O. I. MICIC, H. M. CHEONG, H. FU, A. ZUNGER, J. R. SPRAGUE, [illegible]