. ( ) **224**, . 3, 727 73 (2001)

1.

single-particle electronic (A) 1 3 (k = 0) A 1 6 free-standing fit A accommodate predicts semiconductor-embedded A A 26 (A) 7 $\sim 10^3$ 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 A: The s ng e-part c e prob em

1. The shape, size and composition of the dot are accepted as “input”, [illegible] 3 [illegible]

2. Atoms are relaxed to their strain-minimizing positions [illegible] A 10. [illegible] C_{11}, C_{12}, C_{44} [illegible] A [illegible]

3. The single-particle screened pseudopotential is fit to bulk solids: [illegible] R_n [illegible] α,

$$V + V = \sum_{n,\alpha} V_{\alpha}(r - R_{n,\alpha})\,. \qquad (1)$$

[illegible] V_{α} [illegible] A [illegible] 11, 12. [illegible] A [illegible] 11, 12 [illegible] α [illegible] A [illegible] 13 [illegible]

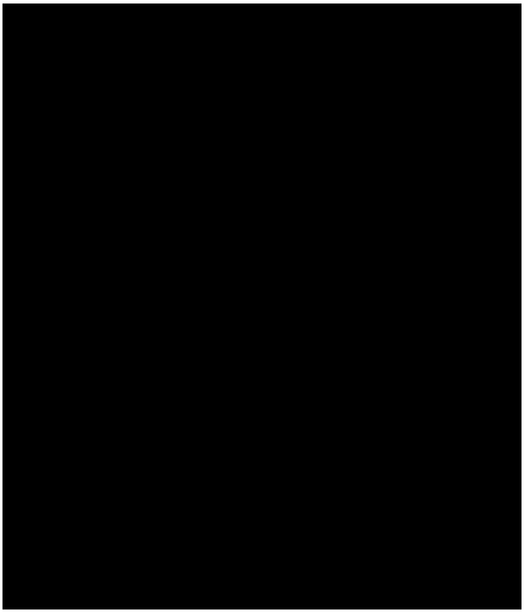
4. The wavefunctions are expanded in plane-waves, [illegible] (Γ [illegible] (Γ) [illegible] 10.

5. The pseudopotential-plane wave Hamiltonian is diagonalized incredibly rapidly [illegible] -N [illegible] ( ) 14, 1 [illegible] 10000 [illegible] 20000 [illegible] 19999 [illegible] (= [illegible] 20000) [illegible] (= [illegible] 20001). [illegible] 14 [illegible] ≈19999 [illegible] (H A)^2. [illegible]

) . ≈10 . ( ) 16 . 1 .

2.2. B: The many-body prob em

1. Inter-electronic integrals are computed numerically: ψ_i J_{ij} K_{ij} 9, 17 , A . 7A . A A7



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

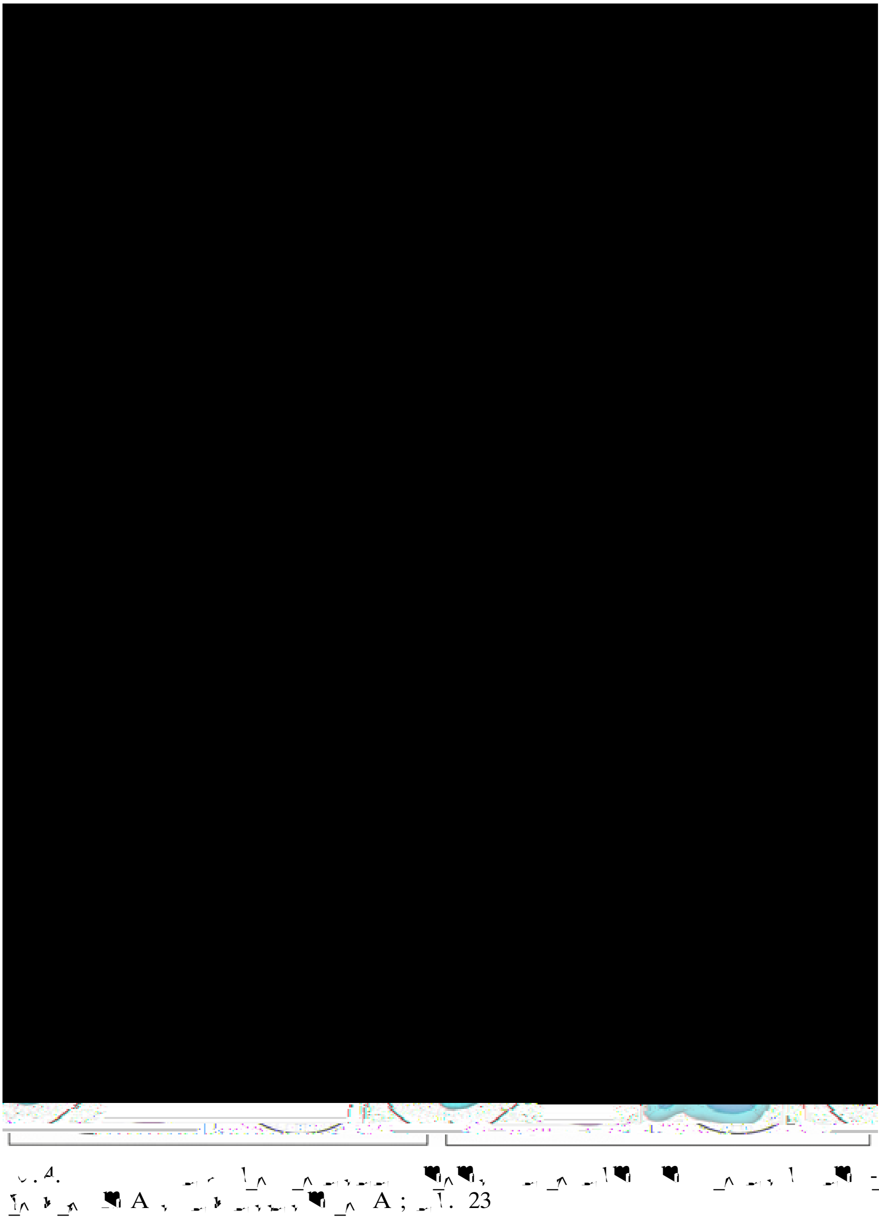
3.2 The ma n accomp shments to-date for the " ntermed ate-energy prob ems"

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

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

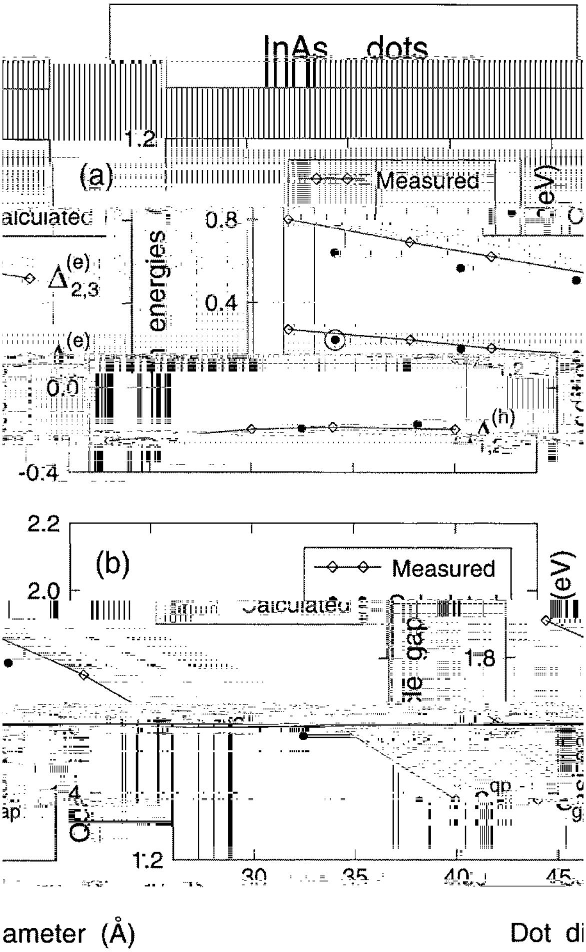
3.3 The ma n accomp shments to-date, for the " ow-energy prob ems"

Established theory of electron hole exchange in dots , 9, 17 . ( ) $\Delta_x \sim \bar{R}^{3}$.



[illegible] A [illegible] A ; [illegible] 23

[illegible] , 9, 17 [illegible] 17 [illegible] 9 [illegible] 9 ([illegible]). [illegible] A [illegible] A [illegible] A , 33 [illegible]



(●) A 30

4. fit predictive

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