

1. \dots A B \dots A B \dots

single-particle electronic

(A)

$(k=0)$ A

6 free-standing fit

date predicts semiconductor-embedded,

26 (A)

10^3 10

many-body description

$(10^3$ $10)$

8 $(-)$ 9

multi-band coupling (A) ,

arbitrary shapes and materials, realistic surface

(multiplet) 10^3 10^5 atoms

2.

A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R, S, T, U, V, W, X, Y, Z, a, b, c, d, e, f, g, h, i, j, k, l, m, n, o, p, q, r, s, t, u, v, w, x, y, z, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100.

2.1 A: T e e - a c e b e

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

2. Atoms are relaxed to their strain-minimizing positions

3. The single-particle screened pseudopotential is fit to bulk solids:

$$V_{\text{w}} + V = \sum_{n,a} V_a(r - R_{n,a}). \quad (1)$$

4. The wavefunctions are expanded in plane-waves,

5. The pseudopotential-plane wave Hamiltonian is diagonalized incredibly rapidly

$$\begin{aligned} & \text{10000} \quad \text{20000} \\ & \text{19999} \quad (= \text{20000}) \quad (= \text{20001}) \\ & \text{1}^4 \quad \approx 19999 \quad \text{(H - A)}^2 \end{aligned}$$

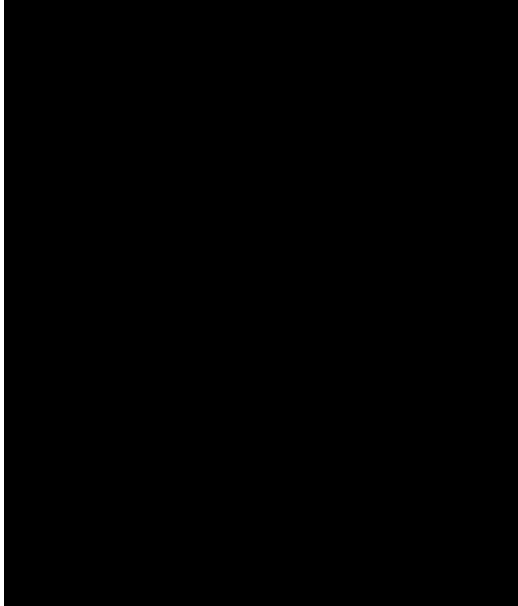
$$\int \psi_i^* \psi_j = \delta_{ij} \approx 10^{-16}$$

2.2. B: Te a , -b d . b e

1. Inter-electronic integrals are computed numerically:

$$J_{ij} = \int \psi_i^* \psi_j \psi_i \psi_j$$

$$K_{ij} = \int \psi_i^* \psi_j \psi_j \psi_i$$



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

3.2 Theoretical studies of electron addition energies in freestanding InAs and CdSe dots

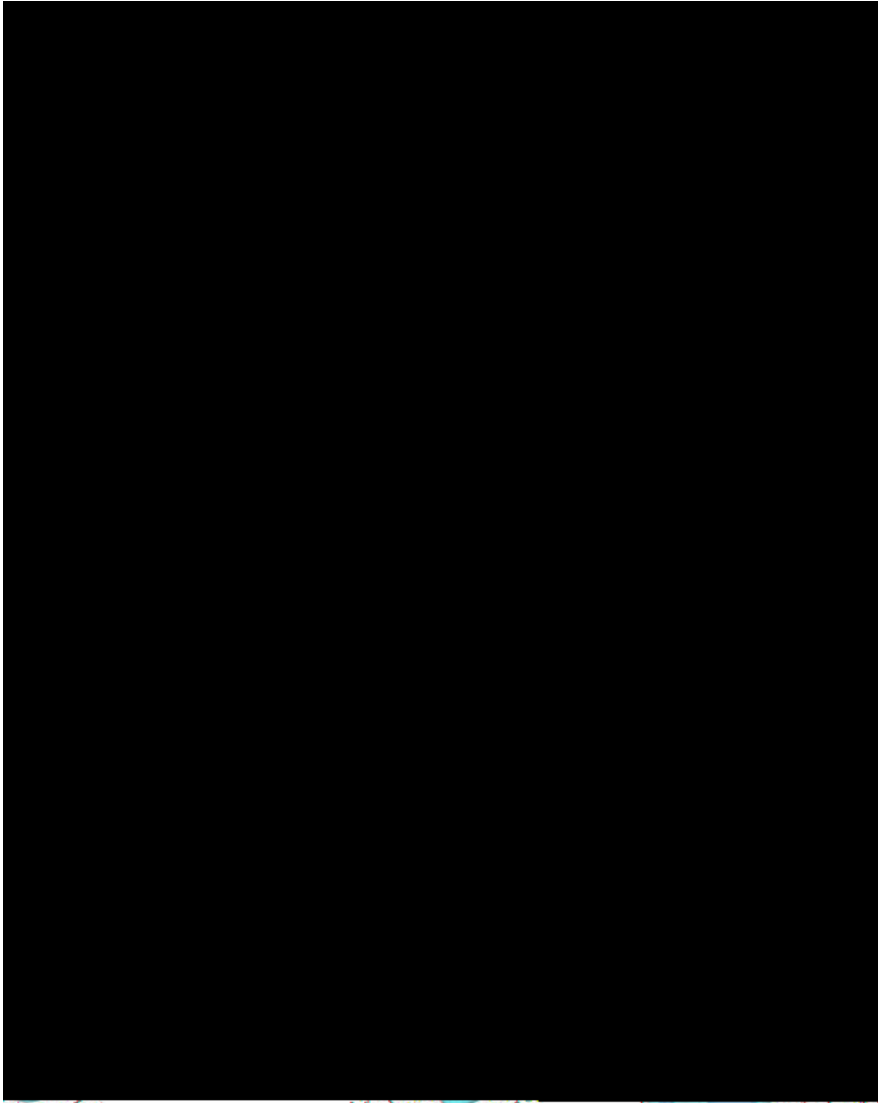
1. Predicted the electron-addition energies in freestanding InAs 30, 31 and CdSe 32 dots,

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

3.3 Theoretical studies of electron-hole exchange in dots

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

$$\Delta_x \sim R^3$$



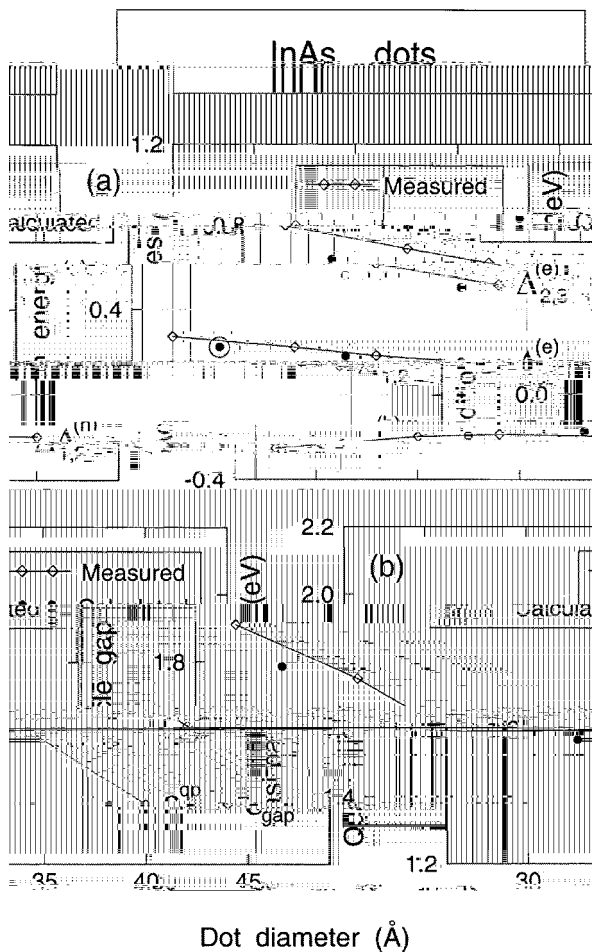
4. A , A ; 23

, 9, 17

17

9 (

A , A , 33



$\Delta_{\text{measured}} = 0.35 \text{ eV}$
 $\Delta_{\text{theoretical}} = 0.35 \text{ eV}$
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