Electronic Phase Diagrams of Carriers in Self-Assembled Quantum Dots: Violation of Hund's Rule and the Aufbau Principle for Holes

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 $\mathcal{L}_{\mathcal{A}}$ the ground-state orbital and spin configurations or holes loaded into self-forms or holes loaded into self-for assembled InAs*=*GaAs quantum dots. We use a general phase-diagram approach constructed from singleparticle pseudopotential and many-particle configuration interaction methods. The predicted hole charging energies agree with recent charging experiments, but offer a different interpretation: we find that while the charging of *electrons* follows both Hund's rule and the Aufbau principle, the charging of *holes* follows a nontrivial charging pattern which violates both the Aufbau principle and Hund's rule.

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\mathbf{D}_{\mathbf{q}}(1/4)I_{\mathbf{q}}, \qquad \mathbf{a} \in \mathbf{q}_{\mathbf{q}} \times I_{\mathbf{q}}.
$$

 $\mathbf{D}_{\mathbf{q}}(M\mathbf{1})$ a, phys $\mathbf{q}_{\mathbf{q}}$ and $\mathbf{q}_{\mathbf{q}}$ and $\mathbf{q}_{\mathbf{q}}$

 $t_{\rm eff}$ the InAs dot with $\Delta t_{\rm eff}$ and 2.5 nm base and 2.5 nm base and 2.5 nm base and 2.5 nm height, $\Delta t_{\rm eff}$ with differences in the addition energies of less than \mathcal{N}_c compared with almost 50% error in 2D-EMA model (despite the fact that two of the addition energies were fitted in the later case $\delta_{p1,p2}$ and $\delta_{p2,d1}$ and ϵ and for different dots are given in Table II and, as shown in $F=\mathbf{F}_{\mathbf{r}}\left(\mathbf{r}_{\mathbf{r}}\right)$ (right), lie close to the center of the predicted of , , , $^{-1}\Delta$, $^2\Delta$ Δ and Λ \sum \sim 1. This indicates the stability of the stabi $\delta_{p1,p2}$ and $\delta_{p1,p2}$ and ρ_{p2} $\delta_{p2,d1}$ due to shape anisotropy of anisotropy of anisotropy of \Box \Box \Box T predicted charging pattern \mathcal{F} shows that the level filling by holes does not follow the Aufbau principle nor the Hund's rules: *d* levels get filled before the second *p* level, despite the fact that the *d* level is energetically more than 3 meV above the second *p* level [26]. The nontrivial hole filling pattern is due to two reasons. First, the large p_1 is the p₂ splitting leads to the *p*₂ level being energetically close to the d_1 level; σ $_{7}^{-}$ δ_{p_2,d_1} is small. In Table II, we list the hole single-particle energy $s_{\rm s}$ s first hole μ first hole $J_{\rm s s}$ for different $J_{\rm s s}$ $\delta_{p_1,p_2} \sim (0.3-0.5) J_{ss}$, $\delta_{p_2,d_1} \sim$
 $(0.2-0.3) J_{ss}$, which differences $J_{ss} = \begin{pmatrix} \frac{\mathbf{D}}{2} & \frac{\mathbf$ *d* level is lower than that between the two *p* levels, therefore the Coulomb energy can overcome the single-particle energy spacing $\delta_{p_2,d_{1/2}}$, leading to the non-Australian charging to the non-Australian charging δ pattern. $\delta_{p_2,d_{1j}}$ is a constant of the set of the s

 $A_{\rm eff}$ important feature of the present theory is not only if χ compatibility with the zero field experimental results but also with the magnetic field dependence obtained in $R = \frac{1}{2}$. In our calculations, the hole single-particle level si p_1 has mixed characters of $L_z = +1$ and $L_z = -1$. state which is k ramers degenerate at $B = 0$ will therefore s_p in opposite direction in the magnetic field. This agrees in the magnetic field. This agree α with the observation of the hole charging $\mathbf{15}$. \overline{p}_2 and \overline{p}_2 and $L_z = +1$. $\overline{L_z} =$ -1 characters and d_1/d_2 and $L_z = +2$ and $L_z =$ -2 characters.

In conclusion, we developed a general phase-diagram approach that classifies the many-particle configurations of $\mathcal{A}_\mathcal{A}$ for electrons and holes in quantum dots in terms of simple electronic and geometric parameters. From these diagrams, we predict that the hole charging sequence presents sur-