\mathcal{L}_{G} is and Alex \mathcal{L}_{G} and \mathcal{L}_{G} and \mathcal{L}_{G} and \mathcal{L}_{G} *National Renewable Energy Laboratory, Golden, Colorado 80401, USA* R_{R} $\frac{1}{6}$ **16** $\frac{200}{100}$ **1** $\frac{1}{200}$

We calculate the excitonic optical absorption spectra of $\mathcal{A}_\mathcal{A}$ self-assembled quantum dots by a self-assembled $\mathcal{A}_\mathcal{A}$ adopting an atomistic pseudopotential approach to the single-particle problem followed by a configuration-particle problem for χ^2 interaction approach to the many-body problem. We find three types of *allowed* transitions that would be naively expected to be forbidden: i transitions that are parity forbidden in simple effective mass models with infinite confinite confinite μ a.g., 1*S-2S*, $1P$ -2*P* but are possible because of finite band of finite band of μ in μ $\frac{1}{2}$ in the hole-to-conduction-band transition-band transition-band transition-band $\frac{1}{2}$ that show an enhanced intensity due to electron-hole configuration mixing with all α We compare these predictions with results of eight-band **k**· calculations as well as recent spectroscopic data. Transitions of types i and ii explain recently observed satellites of the allowed *P*-*P* transitions.

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I. IN OD C ION

In quantum dot spectroscopy, rather simple, idealized the- $\mathbf{C}(\mathbf{x}_k) = \mathbf{C}(\mathbf{x}_k)$ approaches have been applied to discuss which confined interband optical transitions are formally allowed and $w_{\mathbf{x}}$ are formally formally formally for \mathbf{y} rules not to work. We have the mechanisms for failure f been assessed with extensions of the simple models. The simple models \mathcal{P}_c understand these mechanisms demands a high-level ap p is that naturally includes that naturally includes the dots. The dots of the dots of the dots. \mathbb{S} Such approaches to the calculation of the optical properties of the optical properties of the optical properties \mathbb{S} are rare, with eight-band **k**·

tum dot with dot with b/200 $\frac{1}{2}$ and $\frac{1}{20}$ that confines two shells of electron states: 1*Se* ;1*Pe* . The energy of the transitions is shown as a shift $\mathcal{E}(\mathfrak{e})$ $\mathcal{E}(\mathfrak{e})$ $\mathcal{E}(\mathfrak{e})$. Shown as \mathcal{E}_0^e \mathcal{E}_1^h \rightarrow \mathcal{E}_2^e \mathcal{E}_0^h

including the valuence-band maximum VBM states on \mathbb{R}^n \overline{M} considering to considering the VBM states plus the VBM states \overline{M} conduction-band [min](#page-5-1)imum. Higher values of *N* have been also considered.²³

 $\frac{1}{3}$ b/ 252 \rightarrow the larger base size size size size space size space size space space size space tween confined hole states and promotes character mixing. In the state $\frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{2} \frac{1}{2}$ $\mathcal{M}_{\mathcal{F}}$ two-shell dot, the offset energy of this transition with $\mathcal{F}_{\mathcal{F}}$ respect to $1P_{hh}^{-1}P_{e,v}$ 3.0 met_{ry} is a construction with with the observed value. 37 Note that simple models that follow that follow the follow that follow the follow the follow the following the simple models that follow the simple models with the simple models with the simple mo common assumption of unconfined lines assumption of unconfined lines of \mathbf{r}_i the observed feature.

3. $C \rightarrow b$ *feld* ced, *de* ℓ , *ke* ℓ , *a* a *e* ℓ *b dde²<i>k***e** ℓ , **e** ℓ *ke* ℓ **e** *g*, c *e* deg c , Re^2

 $D_{\rm{max}}$, the electron-hole $\mathcal{N}_{\rm{max}}$ interaction, each model interaction, each model model interaction, each model in noexciton state X^0 is a mixture of electron-hole configuration-hole configurationrations \mathbb{R}^3 \mathbb{R}^3 . \mathbb{R}^3 results in enhancement or diminishment of the intensity of the intensity of the intensity of \mathcal{E}_in for bidden transitions in the absorption spectra $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$, $\frac{1}{2}$. These are shown by comparing $\mathbf{r}_s = \mathbf{r}_s$ in $\mathbf{r}_s = \mathbf{r}_s \mathbf{r}_s = \mathbf{r}_s \mathbf{r}_s \mathbf{r}_s = \mathbf{r}_s \mathbf{r}_s$ F_1 , F_2 F_2 vs F_3 F_4 , F_5 F_6 F_7 F_8 include includ ectra

in the atomistic calculation the configuration that χ^2 $\Omega_{\rm C}$ enhanced transition corresponds to a mixture of states to a mixture of states to a mixture of states of states $\Omega_{\rm C}$ $2S_{hh}1S_e$ and *B* instead of a mixture of *H* and *B* and *B* the model [of](#page-3-1) $\overline{5}$ $\overline{5}$ $\overline{5}$ is an and $\overline{D_5}$ the state peak of \overline{r} $D = \sqrt{1 + \frac{1}{2}}$, $\sqrt{1 + \frac{1}{2}}$ a mixture of $D = \frac{1}{2} \int_{0}^{2\pi} F(x,y) dx = 2\pi \int_{0}^{2\pi} F(x,y) dx$

C. Comparison with eight-band kind komparison f **interband optical spectrum**

Other authors have calculated the absorption spectrum of $p(x_1, \ldots, x_{n-1}, x_n) = \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \left| \int$ band **k**· method with cubic symmetry. A comparison with $\overline{\mathbf{U}}$ our atomistic, pseudopotential-based predictions in allowed predictions in all $\overline{\mathbf{v}}$ $I_{\rm eff}$ and $I_{\rm eff}$ as dots shows the following main features. i $O(n^{10} + \epsilon_{\text{max}} + \epsilon_{\text{max}} + \epsilon_{\text{max}} + \epsilon_{\text{max}} + 2S_{hh} - 1S_{e} + \epsilon_{\text{max}} + \epsilon_{\text{max}} + 1S - 1S_{h}$ and $1P-1P$ is consistent with the finding \mathbf{r} finding \mathbf{r} bidden transitions between 1*S*-1*S* and 1*P*-1*P* by Heitz *et al.*, [1](#page-4-2) who calculated the many-body absorption spectrum of absorpti monoexciton in pyramid-shaped nonalloyed InAs/GaAs dots with base length of $d/1/0$ \rightarrow μ μ \rightarrow μ μ \rightarrow μ μ and μ eta_{α}^{2} eta_{α}^{2} eta_{α}^{2} who calculated the many-body absorption spectra of α t_{tot} \sim t_{c} \sim t_{c} \sim $\frac{d}{10}$, *h*/35 and the single-particle calculations of Δt and Δt and Δt i in the case of a pure non-shaped lens-shaped InAs/GaAs dotter in As/GaAs dotter in As/GaAs dotter in As/GaAs do \int 34 d/ 153 \int _{an} h/3⁴ Å. Conversely, other eights-band **k**· plus CI calculations did not predict nominally-forbidden t_{max} [an](#page-4-5)d t_{max} 1*S*-1*S* and 1*P*-1*P*, $\sqrt{t_{\text{max}}}\approx t_{\text{max}}$ *et al.* for all $\epsilon_{\mathbf{a}} = \mathbf{e}_{\mathbf{a}} + \mathbf{e}_{\mathbf{a}} / \mathbf{e}_{\mathbf{a}}$ and $\epsilon_{\mathbf{a}}$ is $\epsilon_{\mathbf{a}}$ with h \sim 4 Å base length unspecified , who found the groups of \sim $t₁$, $t₂$, $t₃$, $t₄$, 1*S*-1*S*, 1*P*-1*P*, $\frac{1}{2}$, 1*D*-1*D*, *without* \cdots γ satellites around transitions $1P$ -1*P*. Similarly, recent called called γ culations by Heitz absorptions absorption spectrum for e small, flat **d** $\frac{1}{3}$ and $\frac{1}{3}$ and $\frac{1}{3}$ monolayers from $\frac{1}{3}$ $\mathcal{F}_{\mathcal{F}}$ satellites are not truncated-pyramid InAs/Ga^R, and $\mathcal{F}_{\mathcal{F}}$ and $\mathcal{F}_{\mathcal{F}}$ eterminations also alcohomology 362*the [etet](#page-5-2)

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