Selection rules for optical transitions in PbSe nanocrystal quantum dots: Drastic effect of structure inversion asymmetry

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We resolve a paradox according to which optical transitions seemingly forbidden in PbSe nanocrystal quantum dots by the parity selection rule exhibit large oscillator strengths in optical absorption. The transitions become allowed if the center of a spherical nanocrystal is shifted away from an atomic site leading to the structure inversion asymmetry. This asymmetry is accounted for within a four-band envelope-function formalism. Transition strengths for various optical transitions are calculated.

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Recently PbSe semiconductor nanocrystals (NCs) have attracted much attention because of highly efficient multiexciton generation and/or carrier multiplication[1,2] which makes them promising for solar-energy conversion applications. Their systematic study began a decade ago when a model based on the effective-mass approximation and assuming spherical shape of NCs was formulated.[3] However, subsequent works[4,5] revealed that some of the optical transitions forbidden by the parity selection rule within this model are in reality among transitions dominating optical-absorption spectra. While no satisfactory explanation of this apparent controversy has been found, the model of Ref. 3 remains to be in the core of various studies addressing optical properties of PbSe NCs.[2,6,7] The aim of the present work is to resolve the above-mentioned controversy.

The *IV-VI* semiconductor compounds such as lead chalcogenides crystallize in a rock-salt lattice. This lattice can be obtained from a simple cubic (sc) lattice with half the period where atoms of the two types are arranged as on a chess board. The Bravais lattice of such a structure has a fcc type. The minima of the conduction band and the maxima of the valence band in lead chalcogenides are located at four equivalent L points of the Brillouin zone.

The genesis of energy bands of IV-VI semiconductor compounds can be explained by the tight-binding approximation taking into account only p atomic orbitals.[8,9] Within this treatment the electron spectrum is constructed by starting with a parent phase having a sc lattice into which the rock-salt lattice is transformed if the neighboring atoms are regarded as equivalent. The difference between the *IV* and *VI* atoms is then taken into account by introduction of the ionicity potential which has the fcc lattice symmetry. At the final stage hybridization of atomic orbitals and the spin-orbit coupling are taken into account.[8,9] As a result, it turns out that the Bloch functions at the extrema of the conduction and valence bands transform according to the odd $L_6^-(L_2')$ and even $L_6^+(L_1)$ irreducible representations of the double group D_{3d} of the L point of the Brillouin zone, respectively (representations of the group D_{3d} neglecting the spin-orbit coupling are shown in the parentheses).

Electron spectrum near the L point taking into account only the two closely lying conduction and valence bands and neglecting band anisotropy can be described by the spherical Dimmock model.[10–12] In this model the electron wave function is written as

$$\hat{\Psi} = \hat{u}|L_6^-\rangle + \hat{v}|L_6^+\rangle, \tag{1}$$

where $|L_6^-\rangle$ and $|L_6^+\rangle$ describe space dependence of the Bloch functions while $\hat{u}(\mathbf{r})$ and $\hat{v}(\mathbf{r})$ are the spinors slowly varying with coordinates and satisfying the equations[13]

$$\begin{bmatrix} \left(\frac{E_g}{2} - \alpha_c\Delta\right) & -iP(\boldsymbol{\sigma}\boldsymbol{\nabla}) \\ -iP(\boldsymbol{\sigma}\boldsymbol{\nabla}) & -\left(\frac{E_g}{2} - \alpha_v\Delta\right) \end{bmatrix} \begin{bmatrix} \hat{u} \\ \hat{v} \end{bmatrix} = E \begin{bmatrix} \hat{u} \\ \hat{v} \end{bmatrix}. \tag{2}$$

Here σ_β ($\beta=x,y,z$) are the Pauli matrices; α_c, α_v, E_g, and P are parameters of the model; and E is the electron energy. These equations imply that the coordinate origin coincides with one of the atoms. Then it follows that Dimmock's Eq. (2) must be invariant under space inversion. This condition is fulfilled if the spinors $\hat{u}$ and $\hat{v}$ are of opposite parities. As the functions $|L_6^\pm\rangle$ are themselves even (odd), the wave function $\hat{\Psi}$ can also be characterized by a certain parity.

Consider a PbSe NC of spherical shape with the center of the sphere on one of the atoms (we will call such a structure *symmetric*). Electron states in this quantum dot (QD) can be characterized by the total angular momentum and parity. One can construct the corresponding solutions of Dimmock's equations and find energy levels of size quantization from the condition of the wave function vanishing at the NC spherical surface. Such consideration was undertaken by Kang and Wise.[3] It is clear that in such a model optical transitions satisfy the parity selection rule.

Note that Dimmock's equations can be rewritten in a basis of Bloch functions representing linear combinations of the functions $|L_6^-\rangle$ and $|L_6^+\rangle$. These Bloch functions would not have a certain parity. Then the only good quantum numbers are the total angular momentum and its projection. When finding electron levels of size quantization in a symmetric spherical QD with the total angular momentum fixed, one would obtain a single dispersion equation[14] instead of two of them (one for each parity) in the paper by Kang and Wise.[3] Of course, both this treatment and the one of Ref. 3 will yield the same energies of size quantization and electron eigenfunctions. But, formally, in addition to the total angular momentum F (and its projection), electron states will be characterized by a single main quantum number (n_c^F or n_v^F)

instead of the parity and a pair of main quantum numbers (one for each parity) in the paper by Kang and Wise.[3] This way of electron-state classification turns out to be more convenient. In Fig. 1 the dependences of energies of several lowest (uppermost) levels of size quantization in the conduction (valence) band on the NC radius are shown. All the parameter values are taken from Ref. 3. For a symmetric structure the transitions $F=1/2$, $n_v^{1/2}=1 \rightarrow F=1/2$, $n_c^{1/2}=2$; $F=1/2$, $n_v^{1/2}=1 \rightarrow F=3/2$, $n_c^{3/2}=1$; $F=1/2$, $n_v^{1/2}=2 \rightarrow F=1/2$, $n_c^{1/2}=1$, and $F=3/2$, $n_v^{3/2}=1 \rightarrow F=1/2$, $n_c^{1/2}=1$ are forbidden by the parity selection rule.

The symmetric QD structure necessarily has unequal numbers of atoms of each type. Indeed, if an atom of a given type is placed at the center of the sphere then its nearest neighbors are of the opposite type, the next-nearest neighbors are again of the same type and so on. In the meantime, it would make the model more flexible if we learn how to change the relative number of atoms of each type within the spherical QD of a given radius. This can be achieved by shifting the center of the sphere along the [111] direction. A shift by the vector $(a/4,a/4,a/4)$, where a is the lattice period, would make the numbers of atoms of each type equal. We will consider a more general case when the center of the sphere is shifted by the vector $(\gamma a, \gamma a, \gamma a)$, where $0 < \gamma \leq 1/4$, with respect to its position in a symmetric structure. This will enable us to address more realistic QD structures while still taking the advantages of QDs with a spherical shape. We will call the resulting structure *asymmetric*. An asymmetric structure with $\gamma \neq 0$ has no center of inversion and is not subject to the parity selection rule.

We will proceed by finding out how solution (1) of Dimmock's Eq. (2) behaves when the coordinate origin is moved to the point $(\gamma a, \gamma a, \gamma a)$. The Bloch functions in the nearly-free-electron model have the form[15,16]

$$\langle \mathbf{r}|L_6^+(L_1)\rangle = \sqrt{\frac{2}{3}}\left[\cos\frac{\pi}{a}(3z-x-y)+\cos\frac{\pi}{a}(3x-y-z)+\cos\frac{\pi}{a}(3y-x-z)\right], \tag{3}$$

$$\langle \mathbf{r}|L_6^-(L_2')\rangle = \sqrt{\frac{2}{3}}\left[\sin\frac{\pi}{a}(3z-x-y)+\sin\frac{\pi}{a}(3x-y-z)+\sin\frac{\pi}{a}(3y-x-z)\right]. \tag{4}$$

The new coordinates are related to the old ones by $\mathbf{r}'=\mathbf{r}-(\gamma a, \gamma a, \gamma a)$. Therefore,

$$\langle \mathbf{r}|L_6^+\rangle = \cos\gamma\pi\,\langle \mathbf{r}'|L_6^+\rangle - \sin\gamma\pi\,\langle \mathbf{r}'|L_6^-\rangle, \tag{5}$$

$$\langle \mathbf{r}|L_6^-\rangle = \sin\gamma\pi\,\langle \mathbf{r}'|L_6^+\rangle + \cos\gamma\pi\,\langle \mathbf{r}'|L_6^-\rangle. \tag{6}$$

We will assume that relations (5) and (6) are valid beyond the nearly-free-electron model. In the meantime the slowly varying envelope spinors are not sensitive to the coordinate change of this scale and continue to satisfy Dimmock's Eq. (2). As a result, the dependence of the wave function on the new coordinates takes the form

$$\hat{\Psi}(\mathbf{r}') = [\cos\gamma\pi\,\hat{u}(\mathbf{r}') - \sin\gamma\pi\,\hat{v}(\mathbf{r}')]\langle \mathbf{r}'|L_6^-\rangle + [\sin\gamma\pi\,\hat{u}(\mathbf{r}') + \cos\gamma\pi\,\hat{v}(\mathbf{r}')]\langle \mathbf{r}'|L_6^+\rangle \equiv \hat{\xi}(\mathbf{r}')\langle \mathbf{r}'|L_6^-\rangle + \hat{\eta}(\mathbf{r}')\langle \mathbf{r}'|L_6^+\rangle. \tag{7}$$

This wave function does not have a certain parity with respect to the change $\mathbf{r}' \rightarrow -\mathbf{r}'$ as the inversion with respect to the point $(\gamma a, \gamma a, \gamma a)$ is not a symmetry operation of the rock-salt lattice. However, as the spinors $\hat{u}$ and $\hat{v}$ satisfy Dimmock's Eq. (2), they must be of opposite parities. For the same reason the electron levels of size quantization in an asymmetric QD have the same energies as the levels in a symmetric QD of the same radius.

The last line of Eq. (7) could be written right away by analogy with Eq. (1). Then we would have to write equations for the spinors $\hat{\xi}$ and $\hat{\eta}$. But there is no need for such equations because the spinors $\hat{\xi}$ and $\hat{\eta}$ are related by Eq. (7) to the spinors $\hat{u}$ and $\hat{v}$ satisfying Dimmock's Eq. (2).

The matrix element of the optical transition between the valence-band state of an asymmetric QD described by the wave function $\hat{\Psi}_v$ and the conduction-band state described by the wave function $\hat{\Psi}_c$ is given by

$$\langle c|\mathbf{ep}|v\rangle = \int d\mathbf{r}[\hat{\xi}_c^\dagger(\mathbf{r})(-i\mathbf{e}\boldsymbol{\nabla})\hat{\xi}_v(\mathbf{r}) + \hat{\eta}_c^\dagger(\mathbf{r})(-i\mathbf{e}\boldsymbol{\nabla})\hat{\eta}_v(\mathbf{r}) + \hat{\xi}_c^\dagger(\mathbf{r})P(\mathbf{e}\boldsymbol{\sigma})\hat{\eta}_v(\mathbf{r}) + \hat{\eta}_c^\dagger(\mathbf{r})P(\mathbf{e}\boldsymbol{\sigma})\hat{\xi}_v(\mathbf{r})], \tag{8}$$

where $\mathbf{e}$ is the vector describing polarization of light and $\mathbf{p}$ is the momentum operator. From Eq. (8) one can see that if the spinors $\hat{\xi}_{c,v}$ and $\hat{\eta}_{c,v}$ have certain parities (which is the case of a symmetric structure) then the parity selection rules hold. The spinors $\hat{\xi}_{c(v)}$ and $\hat{\eta}_{c(v)}$ characterizing an electron state with the total angular momentum F and its projection M in the conduction (valence) band of a QD can be expressed through the spherical spinors[17]

$$\hat{\Omega}_{FM}^{F-1/2}\left(\frac{\mathbf{r}}{r}\right) = \begin{bmatrix} \sqrt{\frac{F+M}{2F}}\,Y_{F-1/2,M-1/2}\left(\frac{\mathbf{r}}{r}\right) \\ \sqrt{\frac{F-M}{2F}}\,Y_{F-1/2,M+1/2}\left(\frac{\mathbf{r}}{r}\right) \end{bmatrix}, \tag{9}$$

$$\hat{\Omega}_{FM}^{F+1/2}\left(\frac{\mathbf{r}}{r}\right) = \begin{bmatrix} -\sqrt{\frac{F+1-M}{2(F+1)}}\,Y_{F+1/2,M-1/2}\left(\frac{\mathbf{r}}{r}\right) \\ \sqrt{\frac{F+1+M}{2(F+1)}}\,Y_{F+1/2,M+1/2}\left(\frac{\mathbf{r}}{r}\right) \end{bmatrix}, \tag{10}$$

as

$$\hat{\xi}_{c,v}(\mathbf{r}) = f_{F-1/2}^{c,v}(r)\hat{\Omega}_{FM}^{F-1/2}\left(\frac{\mathbf{r}}{r}\right) + f_{F+1/2}^{c,v}(r)\hat{\Omega}_{FM}^{F+1/2}\left(\frac{\mathbf{r}}{r}\right), \tag{11}$$

$$\hat{\eta}_{c,v}(\mathbf{r}) = g_{F-1/2}^{c,v}(r)\hat{\Omega}_{FM}^{F-1/2}\left(\frac{\mathbf{r}}{r}\right) + g_{F+1/2}^{c,v}(r)\hat{\Omega}_{FM}^{F+1/2}\left(\frac{\mathbf{r}}{r}\right), \tag{12}$$

where the functions $f_L^{c,v}(r)$ and $g_L^{c,v}(r)$ are the radial functions to be specified later on and Y_{LM} are the spherical harmonics. Substituting these expansions into Eq. (8) one can express the matrix element of an optical transition through a $3j$-Wigner symbol,

TABLE I. Radial functions for various conduction- and valence-band states of electron confined in PbSe QD.

β, n_β^F	$f^\beta_{F-1/2}(r)$	$f^\beta_{F+1/2}(r)$	$g^\beta_{F-1/2}(r)$	$g^\beta_{F+1/2}(r)$
$\beta=c, n_c^F$, is odd $\beta=v, n_v^F$ is even	$\cos\gamma\pi\, A_\beta z^\beta_{F-1/2}(r)$	$-i\sin\gamma\pi\, A_\beta\rho(k_\beta) z^\beta_{F+1/2}(r)$	$\sin\gamma\pi\, A_\beta z^\beta_{F-1/2}(r)$	$i\cos\gamma\pi\, A_\beta\rho(k_\beta) z^\beta_{F+1/2}(r)$
$\beta=c, n_c^F$ is even $\beta=v, n_v^F$ is odd	$i\sin\gamma\pi\, B_\beta\rho(k_\beta) z^\beta_{F-1/2}(r)$	$\cos\gamma\pi\, B_\beta z^\beta_{F+1/2}(r)$	$-i\cos\gamma\pi\, B_\beta\rho(k_\beta) z^\beta_{F-1/2}(r)$	$\sin\gamma\pi\, B_\beta z^\beta_{F+1/2}(r)$

$$\langle c,F',M',n_c^{F'}|\mathbf{ep}|v,F,M,n_v^F\rangle = (-1)^{F-M} e_\mu \begin{pmatrix} F' & F & 1 \\ M' & -M & \mu \end{pmatrix} \langle c,F',n_c^{F'}||\mathbf{ep}||v,F,n_v^F\rangle, \tag{13}$$

where $e_{\pm1}=\mp(e_x \pm ie_y)/\sqrt{2}$, $e_0=e_z$,

$$\langle c,F,n_c^F||\mathbf{ep}||v,F,n_v^F\rangle = \frac{\sqrt{2F+1}}{2\sqrt{F(F+1)}}[I_1(F+1/2,F-1/2)+I_2(F-1/2,F+1/2)+2P(F+1)I_3(F-1/2)-2PFI_3(F+1/2)], \tag{14}$$

$$\langle c,F-1,n_c^{F-1}||\mathbf{ep}||v,F,n_v^F\rangle = -\frac{\sqrt{(2F-1)(2F+1)}}{2\sqrt{F}}[I_2(F-3/2,F-1/2)+I_2(F-1/2,F+1/2)+2PI_3(F-1/2)], \tag{15}$$

$$\langle c,F+1,n_c^{F+1}||\mathbf{ep}||v,F,n_v^F\rangle = \frac{\sqrt{(2F+1)(2F+3)}}{2\sqrt{F+1}}[I_1(F+1/2,F-1/2)+I_1(F+3/2,F+1/2)+2PI_3(F+1/2)], \tag{16}$$

$$I_1(L_1,L_2) = i\int_0^R drr^2\left\{f^{c*}_{L_1}\left[\frac{df^v_{L_2}}{dr}-\frac{L_2}{r}f^v_{L_2}\right]+g^{c*}_{L_1}\left[\frac{dg^v_{L_2}}{dr}-\frac{L_2}{r}g^v_{L_2}\right]\right\}, \tag{17}$$

$$I_2(L_1,L_2) = i\int_0^R drr^2\left\{f^{c*}_{L_1}\left[\frac{df^v_{L_2}}{dr}+\frac{L_2+1}{r}f^v_{L_2}\right]+g^{c*}_{L_1}\left[\frac{dg^v_{L_2}}{dr}+\frac{L_2+1}{r}g^v_{L_2}\right]\right\}, \tag{18}$$

$$I_3(L) = \int_0^R drr^2\{g^{c*}_L f^v_L + f^{c*}_L g^v_L\}, \tag{19}$$

and R is the NC radius.

The spinors $\hat{\xi}_{c,v}$ and $\hat{\eta}_{c,v}$ are related to the spinors $\hat{u}_{c,v}$ and $\hat{v}_{c,v}$ satisfying Dimmock's Eq. (2) via Eq. (7). Requiring that the solutions of Dimmock's equations vanish at the QD surface, one can obtain the radial functions $f_L^{c,v}$ and $g_L^{c,v}$ listed in Table I. They are expressed in terms of the functions

$$z^\beta_L(r) = j_L(k_\beta r) - \frac{j_L(k_\beta R)}{i_L(\kappa_\beta R)} i_L(\kappa_\beta r),$$

$$\rho(k) = \frac{E_g - 2E + 2\alpha_c k^2}{2Pk},$$

where j_L is the spherical Bessel function of order L, i_L is the modified spherical Bessel function of order L, $\beta=c$ for $E>0$, and $\beta=v$ for $E<0$. For any sign of the electron energy k and κ are related to it via

$$k = \sqrt{\Xi+\Lambda}, \quad \kappa = \sqrt{\Xi-\Lambda},$$

where

$$\Lambda = \frac{E(\alpha_v-\alpha_c) - P^2 - E_g(\alpha_v+\alpha_c)/2}{2\alpha_c\alpha_v},$$

$$\Xi = \frac{\sqrt{[E(\alpha_v-\alpha_c) - E_g(\alpha_v+\alpha_c)/2 - P^2]^2 + \alpha_c\alpha_v(4E^2-E_g^2)}}{2\alpha_c\alpha_v}.$$

The dispersion equation may be written as[14]

$$\begin{aligned} &i_{F-1/2}(\kappa R) i_{F+1/2}(\kappa R) j_{F-1/2}(kR) j_{F+1/2}(kR) \\ &\quad\times\left\{E_g^2 - 4E^2 + (k^2-\kappa^2)\left[E_g\frac{\alpha_v+\alpha_c}{2} - E(\alpha_v-\alpha_c)\right]\right\} \\ &\quad + P^2k\kappa[i_{F-1/2}(\kappa R)]^2[j_{F+1/2}(kR)]^2 \\ &\quad - P^2k\kappa[i_{F+1/2}(\kappa R)]^2[j_{F-1/2}(kR)]^2 = 0. \end{aligned}$$

The positive, $E>0$ (negative, $E<0$) roots of this equation correspond to energy levels in the conduction (valence) band of the NC. The normalization constants are given by

$$A_\beta = \left\{\int_0^R drr^2[z^{\beta 2}_{F-1/2}(r) + \rho^2(k_\beta) z^{\beta 2}_{F+1/2}(r)]\right\}^{-1/2},$$

$$B_\beta = \left\{\int_0^R drr^2[z^{\beta 2}_{F+1/2}(r) + \rho^2(k_\beta) z^{\beta 2}_{F-1/2}(r)]\right\}^{-1/2}.$$

The radial functions for the limiting case of a symmetric structure can be obtained from Table I at $\gamma=0$.

Let us consider the case when the incident light is linearly polarized along [111] direction. For illustration purposes, we

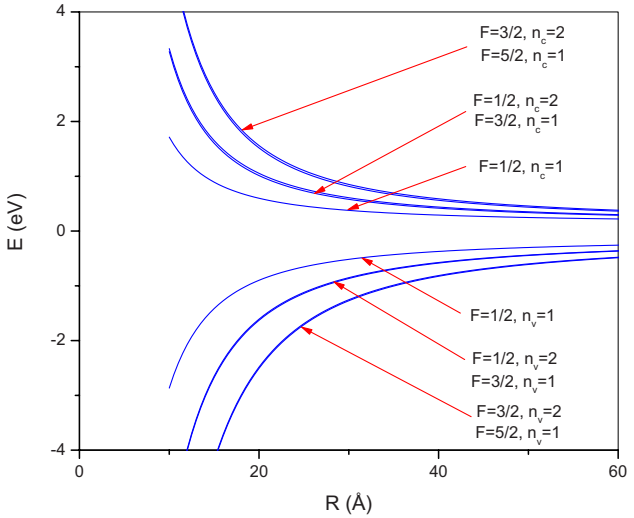

FIG. 1. (Color online) Energy levels of electron confined in PbSe nanocrystal quantum dot as a function of the nanocrystal radius.

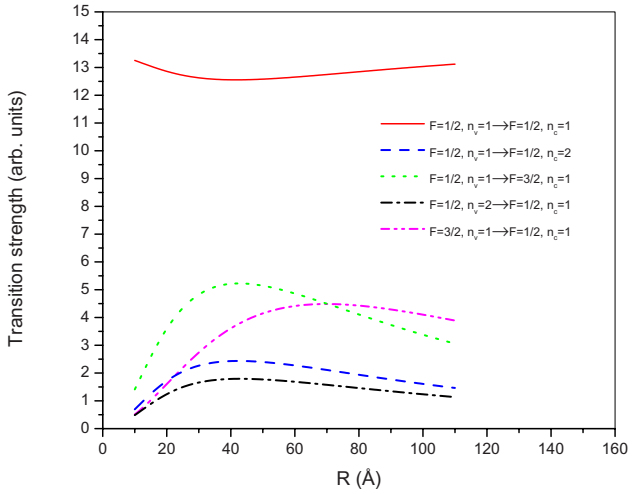

FIG. 2. (Color online) Relative strengths of optical transitions induced by light linearly polarized along [111] direction in an asymmetric quantum-dot structure with $\gamma=3/16$ as a function of the quantum-dot radius.

will take into account only the contribution of the valley with $L=\pi/a(1,1,1)$ to optical absorption. The relative strengths of various optical transitions for an asymmetric QD with $\gamma=3/16$ are plotted in Fig. 2 as a function of the NC radius. One can see that the transitions which would be forbidden for a symmetric structure exhibit appreciable oscillator strengths. The overall trend is as follows. When γ increases from 0 to 1/4 the oscillator strength of the transition $F=1/2$, $n_v^{1/2}=1\rightarrow F=1/2$, $n_c^{1/2}=1$ decreases [as $(\text{const}+\cos 2\pi\gamma)^2$] while the oscillator strengths of all other transitions shown in Fig. 2 increase (as $\sin^2 2\pi\gamma$).

In summary, we have shown how the model of Kang and Wise[3] can be extended in order to account for the observed appreciable oscillator strengths of seemingly forbidden optical transitions.[4,5] One should realize that spherical QD is a model abstraction anyhow. The assumption of sphericity offers a great deal of simplifications and insight. When the center of the sphere is shifted away from the atomic site the QD structure becomes asymmetric with respect to inversion even though the crystal lattice of the bulk semiconductor material possesses such a symmetry, and the parity selection rule no longer applies. This is a manifestation of the so-called structure inversion asymmetry well known in the field of spintronics.[18] There the structure-induced asymmetry can lead to appearance of linear in quasimomentum spin-dependent terms in the electron Hamiltonian. In our case the shift of the center of the sphere away from an atomic site along the high-symmetry [111] direction leads to a change in the ratio of the numbers of atoms of each type within the spherical QD. Therefore, our extension of the model by Kang and Wise[3] accounts for a larger variety of QD realizations. In a real sample containing ensemble of monodisperse QDs all of the QDs can be characterized by the same certain value of the parameter of asymmetry γ or, alternatively, QDs with different values of γ can be present in a given sample.

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