# Photon tunneling into a single-mode planar silicon waveguide

**Liping Fang,[1,*] Kian S Kiang,[2] Nicholas P Alderman,[3] Lefteris Danos,[4] and Tom Markvart[1]**

[1]*Solar Energy Laboratory, University of Southampton, Southampton SO17 IBJ, UK.*

[2]*Electronics and Computer Sciences, University of Southampton, Southampton SO17 IBJ, UK.*

[3]*Department of Chemistry, University of Ottawa, Ottawa K1N 6N5, Canada.*

[4]*Department of Chemistry, University of Lancaster, Lancaster LA1 4YB, UK.*

[*]*liping.fang@outlook.com*

**Abstract:** We demonstrate the direct excitation of a single TE mode in 25 nm thick planar crystalline silicon waveguide by photon tunneling from a layer of fluorescent dye molecules deposited by the Langmuir-Blodgett technique. The observed photon tunneling rate as a function of the dye-silicon separation is well fitted by a theoretical tunneling rate, which is obtained via a novel approach within the framework of quantum mechanics. We suggest that future ultrathin crystalline silicon solar cells can be made efficient by simple light trapping structures consisting of molecules on silicon.

## 1. Introduction

Effective capture of sunlight by semiconductors - particularly silicon - represents one of the great challenges to photovoltaics today. Statistical light trapping techniques based on surface texturing [1] are now commonplace in commercial solar cells (see, for example, [2]). A detailed balance treatment of light trapping in thin films was given in [3] showing that significant enhancements in absorption are possible even when the thin film acceptor only supports a limited number of waveguide modes. Other techniques involve photoexcitation enhancement by exploiting the interaction of a semiconductor with a dipole near the surface. Much work is currently under way to implement such techniques with the use of plasmonics (see, for example, [4]).

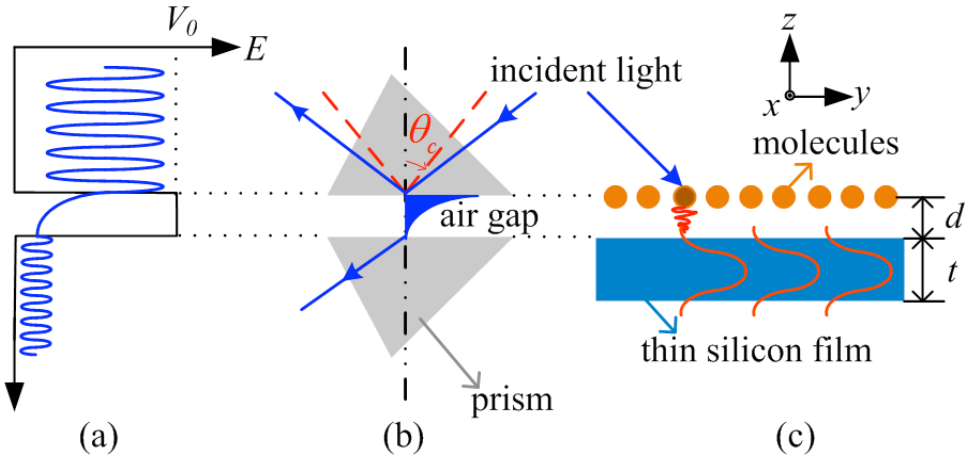


Fig. 1. (a) Quantum tunneling through a potential barrier (b) Photon tunneling through an air gap between two prisms (c) Photon tunneling into thin silicon film.

In this paper we report efficient injection of photons directly into a single mode of a thin silicon waveguide via the interaction of molecules on the surface with the evanescent field. Due to the similarity with frustrated total internal reflection [5] (observed more than a century ago [6]) we have termed this effect photon tunneling, through the potential barrier which confines photons inside the high refractive index material by total internal reflection (Fig. 1) (see also [7]). In our system, we have simply replaced the exciting prism by fluorescent molecules.

## 2. Calculation of photon tunneling rate

The tunneling rate for photons emitted by the molecular dipole into a waveguide mode can be conveniently determined theoretically by the application of the Golden Rule:

$$\gamma_{pt} = \frac{2\pi}{\mathrm{h}^2} \sum_{k_x,k_y} \left| \boldsymbol{\mu} \mathbf{g} \mathbf{E}_k \right|^2 \delta(\omega - \omega_k) \qquad (1)$$

where $\mathrm{h}$ is the reduced Planck's constant, $k_x$ and $k_y$ are the wavenumber components in the $x$ and $y$ directions, $\boldsymbol{\mu}$ is the transition dipole moment, $\mathbf{E}_k$ is the electric field of the trapped mode labelled by the collection of quantum numbers $(k_x, k_y, \boldsymbol{\mu})$, and normalized by:

$$\int \varepsilon_0 \varepsilon_r \left| E_k \right|^2 dV = \mathrm{h}\omega / 2 \qquad (2)$$

where $\varepsilon_0$ is the permittivity of vacuum, $\varepsilon_r$ is the relative permittivity (a function of the $z$ coordinate perpendicular to the waveguide) and $\omega$ the frequency. The summation in Eq. (1) is carried out over the manifold of trapped modes related by cylindrical symmetry, on a shell defined by the characteristic equation for the waveguide mode:

$$\kappa = 2k_{2z}t - 4\phi_{21} = 2m\pi \tag{3}$$

where $\kappa$ is the "round trip" phase shift of the trapped wave, $t$ is the waveguide thickness, $\phi_{21}$ is the phase shift on reflection from the interface between media 1 and 2, and $m$ is an integer. Here we have assumed, for simplicity, that the waveguide is symmetric.

Replacing the summation in Eq. (1) by an integral and transforming to polar coordinates $(k_\rho, \phi)$ gives:

$$\gamma_{pt} = \frac{A}{\mathrm{h}^2}\left\langle \cos^2(\theta)\right\rangle \int_0^\infty dk_\rho k_\rho \left|\mu\right|^2 \left|E_k\right|^2 \delta(\omega - \omega_k) \tag{4}$$

where $k_\rho = \sqrt{k_x^2 + k_y^2}$, $\phi$ is the angle between $k_x$ and $k_y$, $A$ is the mode area, we inserted the density of states $A/(2\pi)^2$ in the $k_x k_y$ plane, and defined the orientation averaging factor:

$$\left\langle \cos^2(\theta)\right\rangle = \frac{1}{4\pi}\int d\Omega \cos^2(\theta) \tag{5}$$

where $\theta$ is the angle between $\boldsymbol{\mu}$ and $\mathbf{E}_k$ and $d\Omega$ denotes an element of the solid angle. The factor $\left|\mu\right|^2 \left|E_k\right|^2$ in Eq. (4) can be taken outside the integral and bearing in mind that the integration is carried out on the shell of $\kappa = constant$, the remaining integral (which effectively gives the density of states of the trapped mode) can be evaluated by standard rules for the delta function:

$$\gamma_{pt} = \frac{A}{\mathrm{h}^2}\left\langle \cos^2(\theta)\right\rangle \left|\mu\right|^2 \left|E_k\right|^2 k_\rho \left(\frac{\partial k_\rho}{\partial \omega}\right)_{\kappa = const} \tag{6}$$

Equation (6) represents the main result for the tunneling rate into the trapped mode. In practical calculations it may be simpler to evaluate the partial derivative with the use of Euler's cyclic relation (see, for example, [8]):

$$\left(\frac{\partial k_\rho}{\partial \omega}\right)_{\kappa=const} = -\frac{\left(\frac{\partial \kappa}{\partial \omega}\right)_{k_\rho=const}}{\left(\frac{\partial \kappa}{\partial k_\rho}\right)_{\omega=const}} \tag{7}$$

giving for the photon tunneling rate in Eq. (4):

$$\gamma_{pt} = \gamma_0 \left\langle \cos^2(\theta) \right\rangle \frac{3\pi}{k_1} \frac{|k_{1z}| k_{2z}^2}{(k_2^2 - k_1^2)(t|k_{1z}| + 2)} \exp(-2|k_{1z}| d) \tag{8}$$

where $\gamma_0$ is the spontaneous emission rate of a dipole in a homogeneous space with refractive index $n_1$: $\gamma_0 = |\mu|^2 n_1 k_0^3 / (3\pi h \varepsilon_0)$, $k_0 = \omega / c$, $c$ is the speed of light, $k_i = n_i k_0$, $k_{iz} = \sqrt{k_i^2 - k_\rho^2}$, and $d$ is the dipole-waveguide separation.

The analytical expression shown in Eq. (8) can also be obtained by complex variable analysis of the pure classical theory developed by Chance, Prock and Silbey (CPS) [9] in the complex wavenumber plane: the rate of photon tunneling to a waveguide mode can be calculated analytically from the contribution of the related pole (of the Fresnel reflection coefficients) to the integral in the CPS model.

**3. Experiments for demonstation of photon tunneling**

Photon tunneling can also be demonstrated experimentally by revisiting the early investigations of energy transfer between molecules and metal by Kuhn [10], Drexhage [11] and colleagues. The comprehensive classical theory developed by CPS can be used to fit the experimental results for the fluorescence lifetime of the $Eu^{3+}$ ions doped in Langmuir-Blodgett (LB) monolayer at different distance to the surface of gold, silver and copper obtained by Drexhage.

In our experiments we have deposited different thicknesses of LB film onto a 25 nm (±5 nm) crystalline silicon layer (fabricated by a series of wet oxidation and HF etching cycles of a silicon-on-insulator wafer with buried oxide thickness of 1000 nm); the last LB bilayer is doped with a carbocyanine dye (1,1'-Dioctadecyl-3,3,3',3'-Tetramethylindocarbocyanine perchlorate). This dye is commonly available and often used as tracers in tissues and cells. It has been studied extensively in the

past by Kuhn [10] and its optical properties are well known. When mixed with stearic acid, this dye can be deposited as stable LB monolayers and it exhibits a high extinction coefficient and a high fluorescence quantum yield.

The dye-silicon separation was controlled by depositing a spacer layer, which was made of different numbers of pure stearic acid LB monolayers, between the dye molecules and the substrate. The thickness of this spacer film has been measured by variable angle spectroscopic ellipsometry, and the error estimated was 0.2 nm.

The fluorescence lifetime of the dye as a function of distance from silicon was measured by time-resolved fluorescence. The dye molecules were excited by a diode laser emitting at the wavelength of 485 nm, and the fluorescence signals were recorded at the peak emission wavelength of the dye molecules, i.e. 566 nm.

For reference, we have also done similar experiments on glass, bulk silicon and copper (sputtered on silicon wafers) substrates. More detailed experimental procedures could be found in our previous publications [12-14], and we only show the results here.

**4. Results and discussion**

Figure 2 shows the measured fluorescence lifetime results (shown by symbols, and has been normalized to the lifetime measured from a glass substrate reference sample $\tau_0$ = 2.1±0.1 ns) and the related modelling results (shown by curves) by CPS for a horizontal electric dipole; an orientation established from a number of previous results [12-14]. It is seen from Fig. 2 that the modeling results fit well with the measured results.

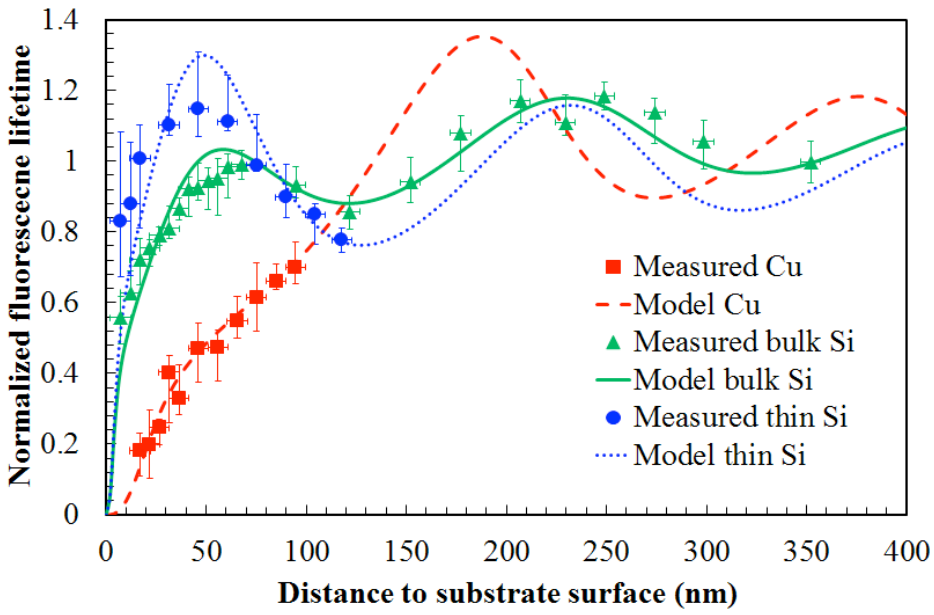


Fig. 2. Fluorescence lifetime versus distance to related substrate.

The difference of the lifetime when the dipole is deposited on different substrates is due to the distinct optical modes that different substrates support when interacting with the molecular dipole. The interaction of a dipole moment with the copper surface is dominated by a surface plasmon mode and lossy surface waves [15]. A dipole on silicon interacts optically to bring about photon tunneling which is considered in this paper. At shorter distances the dipole near field interacts with the near field of the dipole moment of the electron-hole transitions in the semiconductor (not dissimilar to the Förster resonance energy transfer interaction between molecules) which will be discussed in a separate publication. When the dipole-substrate distance is large, the fluctuation of lifetime can be viewed as interference of the source wave of the molecular dipole and its reflected wave from the surface of the substrate.

The classical CPS model is comprehensive, but it hides the key physical process of fluorescence near thin silicon films such as photon tunneling. We demonstrate this process by the comparison of the observed and modeled photon tunneling rates in Fig. 3. The observed photon tunneling rate (yellow dots in Fig. 3) was obtained by subtracting the emission rate into the classically allowed photon states (which can be obtained simply by accounting interference of the source wave of the molecular dipole

and its reflected wave from the interface [10] , shown by dashed blue curve in Fig. 3) from the measured total damping rate (inverse fluorescence lifetime), while the modeled photon tunneling rate (solid red curve in Fig. 3) was calculated from Eq. (8). Here we set $\langle \cos^2(\theta) \rangle = 1/2$ since, in the case of a horizontal electric dipole, both $\boldsymbol{\mu}$ and $\mathbf{E}_k$ lie in the $xy$ plane. It is seen from Fig. 3 that the modeled results show good agreement with the measured results.

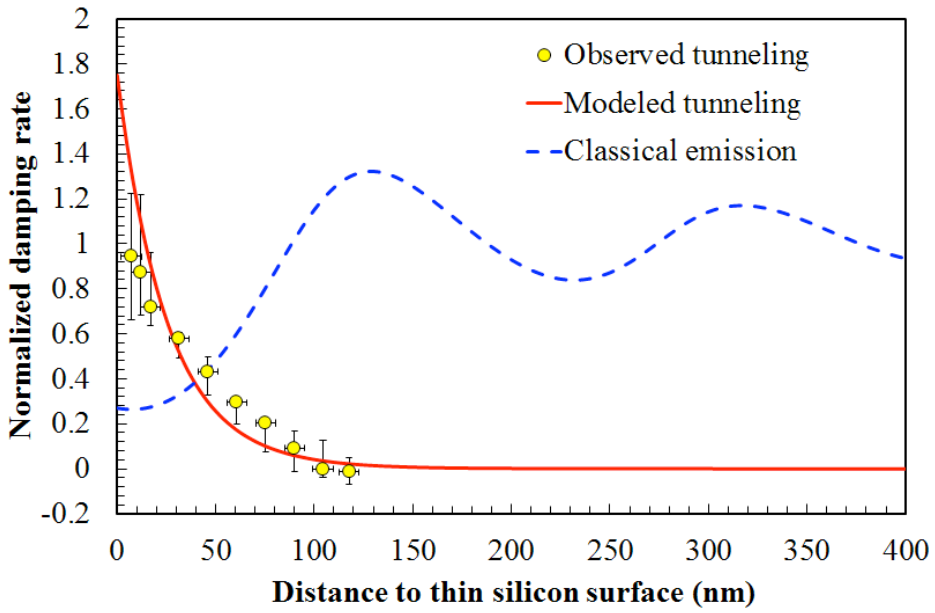


Fig. 3. Comparison of observed and modeled photon tunneling rates.

When the dye-silicon distance approaches zero, strong quenching of fluorescence occurs (see Ref. [12-14]). Thus in time-resolved fluorescence measurements, strong noise signal in the fluorescence decay curves affects the accurate extraction of the fluorescence lifetime results. This is the possible reason for the deviation of the modeled and the measured tunneling rate at short dye-silicon separations.

## 5. Conclusion

In this paper we have demonstrated that fluorescent molecules can couple incident light into the underlying thin silicon film as trapped modes via photon tunneling. This can be perceived as the first step towards the fabrication of efficient ultrathin crystalline silicon solar cells, made possible by the direct coupling of the silicon waveguide modes with the excited states of molecules on silicon. Based

on the ratio between the tunneling rate and the rate of fluorescence emission by the molecules, we estimate that some 70% of photons emitted by the dye molecule in our experiment are injected into the waveguide mode in silicon by tunneling when the molecule-silicon distance is 30 nm. Ultimately, the potential absorption enhancement by light trapping has to include also "reverse" tunneling and will be given by the relevant densities of states (see also ref. [3]). Based on the results of this paper we hope to revisit this topic in a subsequent publication.

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