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## A theoretical study on photocatalytic fuel cell

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### Abstract

This paper presents a theoretical study which investigates the detail potential loss within photocatalytic fuel cell (PFC). Ohmic loss in PFC contributes to 24% potential loss since the large electrical resistance of semiconductor. It is found that Schottky barrier height plays an important role on performance of PFC, and Schottky barrier height of 0.6 eV is preferred for PFC operation. Moreover, current will be enhanced with the activity of photocatalyst increasing.

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Keywords: photocatalytic fuel cell, theoretical model

### 1. Introduction

Photocatalytic fuel cell (PFC) is a kind of photoelectrochemical cell that treats pollutants in wastewater along with generating electricity simultaneously [1, 2]. The light induced electrons and holes are used to produce current and decompose pollutants separately. In PFC, with rapid remove of induced electrons in photoanode, recombination of electron-hole pair, which restricts performance of photocatalytic reaction, will be inhibited. In this work, a theoretical model was implemented. Each potential loss within OFC was classified, and parameter analyses were carried out and discussed in detail.

### 2. Methodology

#### 2.1 Physical problem statement

In this work, a PFC which consists of TiO<sub>2</sub> coated fluorine doped tin oxide (FTO) glass as photoanode couples with gas diffusion electrode (GDE) as cathode was studied. The working principle is shown in Fig. 1. In anode, organic molecules are oxidized by hydroxyl radicals along with generation of protons. The excited electrons transfer to the cathode through external circuit driven by the potential difference between anode and cathode, and takes part in the ORR together with protons. The reactions are summarized as follow [3, 4]:

In anode



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In cathode

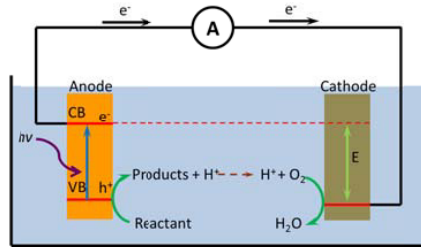
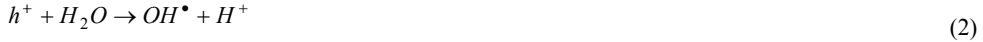


Fig. 1. Working principle of PFC

### 2.2 Theoretical model

In PFC, four parts of potential loss contribute to the whole voltage drop, which occur at anode, cathode, electrolyte and concentration loss.

$$V = E - \eta_a - \eta_c - \eta_e - \eta_{con} \tag{6}$$

At anode, the voltage drop consists of two components, the activation loss at TiO<sub>2</sub>/electrolyte and the electron transfer loss from TiO<sub>2</sub> to FTO glass.

$$\eta_a = \eta_{a,act} + \eta_{a,trans} \tag{7}$$

Like anode, cathode loss in potential is also constitutive of activation and transfer loss. Since the electrical resistance of cathode is quite low (lower than  $1 \times 10^{-4} \Omega \text{ m}$  of carbon electrode), the electron transfer loss was neglected. The potential loss in electrolyte is known as ohmic loss which can be determined by ohmic theory. Therefore, eq. 6 can be rewritten into

$$V = E - \eta_{a,act} - \eta_{a,trans} - \eta_{c,act} - \eta_{ohmic} + \eta_{con} \tag{8}$$

The activation losses at either anode or cathode can be given from the Butler-Volmer equation[5]

$$\eta_{act} = 2RT/(nF) \sinh^{-1}(j/2j_{0,i}) \tag{9}$$

The transfer loss from TiO<sub>2</sub> to FTO glass can be determined by the thermionic-emission theory[6]

$$j = A^* T^2 \exp[-q\phi_b/(kT)] [\exp(q\eta_{trans}/(kT)) - 1] \tag{10}$$

The concentration loss caused by mass transfer limiting near electrode surface can be calculated through mass diffusion flux from bulk solution to reaction surface, and it differs from various operation conditions like stirring, continuous adding of reactants. Herein, sufficient supply of reactant was assumed and the concentration loss is neglected.

All the involved parameters for model input are listed in Table 1.

Table 1 Key input parameters

Parameter	Intendment	Unit	Value	Refs.
$h^+$	Hole	-	-	-
$e^-$	Electron	-	-	-
$\eta$	Overpotential	V	-	-
$E$	Equilibrium potential	V	0.9	Assumed

$n$	Number of transferred electron	-	1	Assumed
$F$	Faradic constant	C mol <sup>-1</sup>	96485	-
$R$	Universal constant	J K <sup>-1</sup> mol <sup>-1</sup>	8.3145	-
$T$	Temperature	K	298	-
$j$	Local current density	mA cm <sup>-2</sup>	-	-
$j_{0,a}$	Exchange current density of anode	mA cm <sup>-2</sup>	$1 \times 10^{-4}$	Assumed
$j_{0,c}$	Exchange current density of cathode	mA cm <sup>-2</sup>	$3.1 \times 10^{-8}$	[7]
$A^{\sim}$	Richardson constant of TiO <sub>2</sub>	A m <sup>-1</sup> K <sup>-2</sup>	$6.71 \times 10^9$	[6]
$\varphi_b$	Schottky barrier height	eV	-	-
$i$	a for anode, c for cathode	mA cm <sup>-2</sup>	$8 \times 10^{-4}$	Assumed
$q$	Charge of electron	C	$1.6 \times 10^{-19}$	-

### 3. Results and discussion

#### 3.1 Each potential loss in PFC

Each potential loss is plotted in Fig. 2a, it is found that activation loss at anode and cathode dominates the potential loss. Taking into consideration that the resistance of semiconductor is relatively large, the contribution of ohmic loss reach as high as 24% of the total loss. Electron transfer loss is much smaller than other ones in this occasion. However, as indicated in Fig. 2b, transfer loss increases significantly with Schottky barrier height rising which results from fast electrons transfer through the interface between TiO<sub>2</sub> and FTO glass.

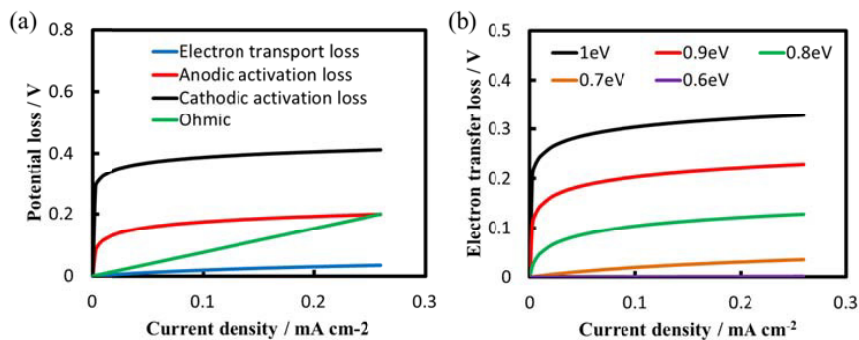


Fig. 2. (a) Each potential loss against current density; (b) electron transfer loss of different Schottky barrier height

#### 3.1 Potential effects on PFC performance

In PFC, the activation loss at anode is related to the activity of photocatalyst which can be expressed by parameter of exchange current density, while the transfer loss of electrons is only related to properties of photocatalyst. As shown in Fig. 3a, the current density increases with anodic exchange current rising. Therefore, enhancement in activity of photoanode is a rapid method to improve the performance of PFC. The influence of Schottky barrier height on cell performance is given in Fig. 3b. Reduction in Schottky barrier height leads to a significant improvement in current density until 0.6 eV, which owes to lower electron transfer resistance within semiconductor. But further improvement in Schottky barrier height affect little on performance as indicated in Fig. 1b that the transfer potential loss nearly comes to zero.

### 4. Conclusion

In this paper, a theoretical study was conducted to investigate the potential loss of PFC. The potential loss occurs at the interface of semiconductor/electrode can be a dominate part among losses. Photoanode with Schottky barrier height of 0.6 eV is preferred. Photocatalyst with high activity which presents high exchange current density is needed to improve the performance.

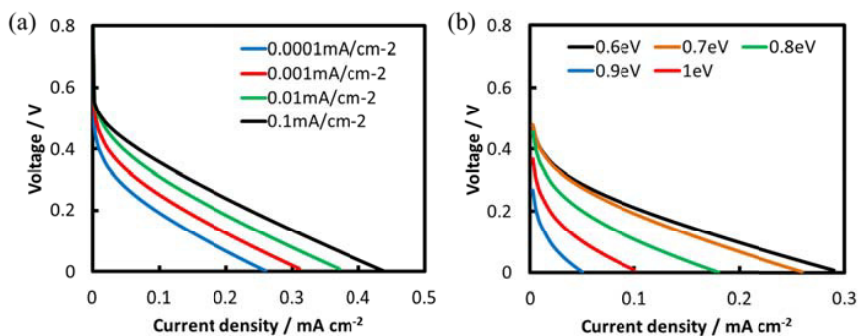


Fig. 3. (a) J-V curves of various anodic exchange current density; (b) J-V curves of various Schottky barrier height

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## Biography

Hao Zhang is a PhD student from East China University of Science and Technology. During his PhD study, he worked as a Research Assistant in Ability R&D Energy Research Center, City University of Hong Kong for 10 months. His research interests focus on microfluidic technology for energy conversion and sustainable energy.