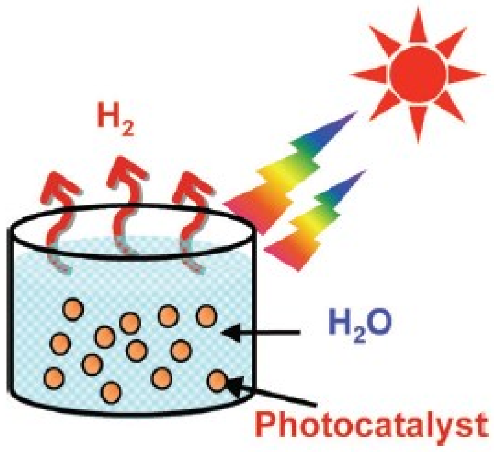
ĐẠI HỌC QUỐC GIA TP. HỒ CHÍ MINH

TRƯỜNG ĐH KHOA HỌC TỰ NHIÊN

KHOA KHOA HỌC VÀ CÔNG NGHỆ VẬT LIỆU



Chương 1– Thiết lập các phương trình tốc độ động học Quang xúc tác

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Giới thiệu

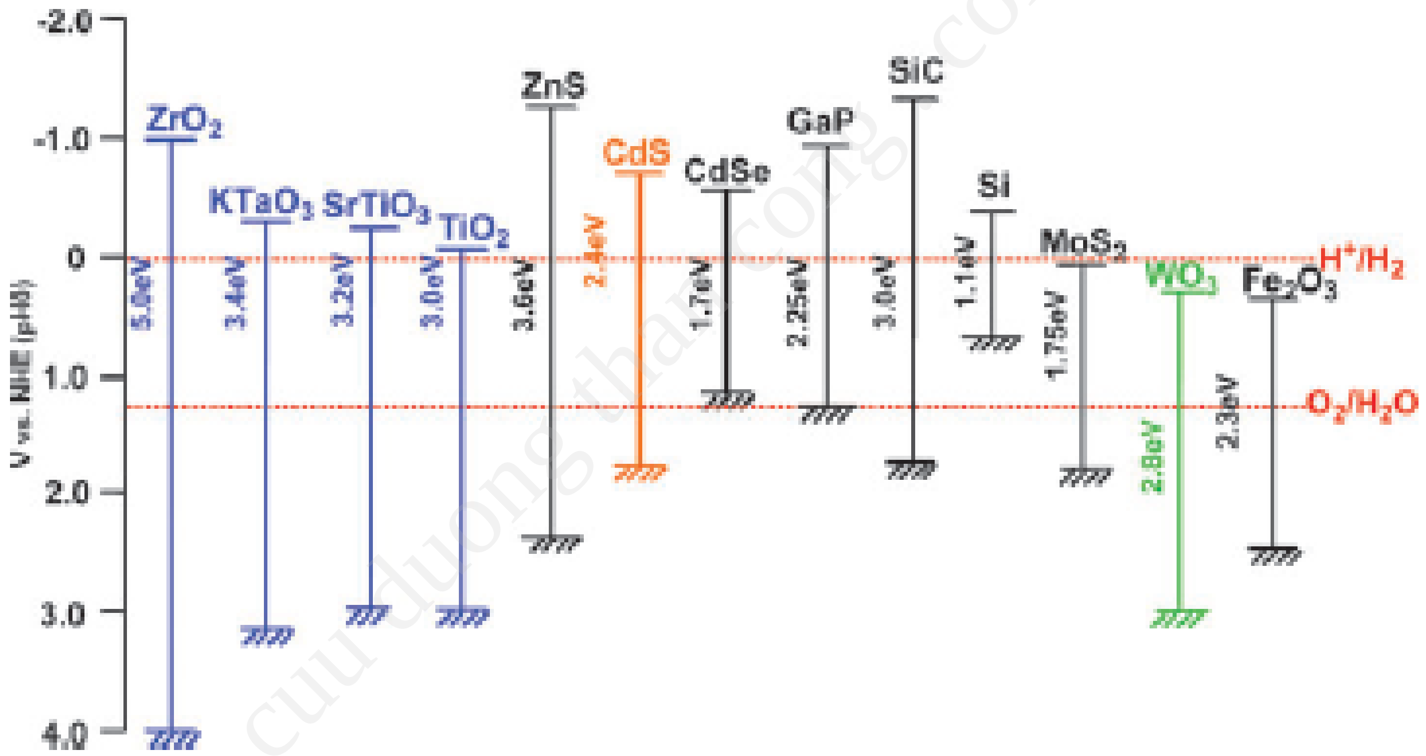

Fig. 6 Relationship between band structure of semiconductor and redox potentials of water splitting.[5]

$$TiO_2 \xrightarrow{h\nu} e^- + h^+ \quad (1\text{-}2)$$

Electron transfer from the adsorbed substrate (RX_{ad}), adsorbed water or the OH_{ad} ion, to the electron-hole.

$$h^+ + RX_{ad} \rightarrow RX^+_{ad} \quad (1\text{-}3)$$

$$h^+ + H_2O_{ads} \rightarrow OH^\bullet_{ads} + H^+ \quad (1\text{-}4)$$

$$h^+ + OH^-_{ad} \rightarrow OH^\bullet_{ad} \quad (1\text{-}5)$$

The third step is of great importance, mostly because of the high concentrations of OH^-, given water dissociation into ions.

$$H_2O \rightarrow OH^-_{ad} + H^+ \quad (1\text{-}6)$$

Molecular oxygen acts as an acceptor species in the electron-transfer reaction.

$$e^- + O_2 \rightarrow O_2^- \quad (1\text{-}7)$$

Super-oxide anions, (equation 1-7), can subsequently be involved in the following reactions.

$$O_2^- + H^+ \rightarrow HO_2^\bullet \quad (1\text{-}8)$$

$$H^+ + O_2^- + HO_2^\bullet \rightarrow H_2O_2 + O_2 \quad (1\text{-}9)$$

Photoconversion of hydrogen peroxide gives more $OH^{\bullet}$ free radical groups.

$$H_2O_2 + h_v \rightarrow 2OH^{\bullet} \tag{1-10}$$

Finally, $OH^{\bullet}$ radicals oxidize organic adsorbed pollutants (RX_{ad}) onto the surface of the titanium dioxide particles.

$$OH^{\bullet}_{ad} + RX_{ad} \rightarrow Intermediate \tag{1-11}$$

The $OH^{\bullet}$ radicals, as described by equation (1-11), are very reactive and attack the pollutant molecule to degrade it into mineral acids including carbon dioxide and water (Al-Ekabi *et al*., 1993).

Adsorption isotherm

The Langmuir-Hinshelwood kinetic adsorption equilibrium isotherms

$$Q_e = \frac{Q_m K_L C_e}{1 + K_l C_e} \qquad (1a)$$

$$\frac{1}{Q_e} = \frac{1}{Q_m K_L C_e} + \frac{1}{Q_m} \qquad (1b)$$

where Q_e is the adsorbed chemical concentration per weight of adsorbent at equilibrium ($mg.g^{-1}$),
C_e is the final equilibrium solution concentration ($mg.l^{-1}$),
K_L is the free energy Langmuir adsorption constant ($mg.l^{-1}$),
and Q_m is the maximum adsorption capacity ($mg.g^{-1}$)

Photolytic reaction kinetics

$$[OC] + h\upsilon \xrightarrow{\Phi I} [OC]_{oxid} \qquad (2)$$

where ϕ and I, are the quantum yield of the reaction and the radiation intensity, respectively

$$V\frac{dC_o}{dt} = \left[\sum_k V_{o,k} R_k\right] W_{ir} \qquad (3)$$

C_o is the concentration of a singular analyte compound, $V_{o,k}$ is a dimensionless stoichiometric coefficient for the compounds involved in reaction step, k and R_k being the rate of photo-conversion of step k based on the unit weight of irradiated catalyst, W_{ir}.

$$r_1 = \frac{V}{W_{ir}} \frac{dC_o}{dt} = \sum_k V_{o,k} R_k \qquad (4)$$

The consideration of Eqs. (3) and (4) leads to the advancement of the photocatalytic conversion rate models into a format that is expressed in Eq. (5).

$$\frac{dC_o}{dt} = \frac{-k_o^m C_o}{1 + \sum_{j-1}^{n} C_j K_j} \qquad (5)$$

where k_o represents the kinetic constants for the o specie and K_j is the adsorption constant for the species j or any other species present

The end!

Thank you for your attention