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研究課題名(和文) 論理的分子設計により、効率的な光電変換出来る近赤外色素の安定性を解明

研究課題名(英文) Elucidation of Stability of NIR Dyes Capable Efficient Photo-conversion by Logical Molecular Design

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研究成果の概要(和文)：近赤外色素の効率的な光子収集性と結合安定性向上のための分子構造の提案を目指し、様々なアンカー基を有する新しい色素の設計開発を、理論的アプローチと実験的アプローチを組み合わせで行った。分子軌道計算に基づく理論エネルギーバンドダイアグラムの予測のための新しい手法を提案し、実験的に求めた値と良好な一致を示すことを確認した。結合安定性と光子収集性の向上のため、それぞれ異なる2種類のアンカー基を有する色素を設計開発した。シアノアクリル酸のみを有する色素と比較し、光子収集性の向上だけでなく、約550倍強い結合性を示す、アクリル酸とホスホン酸の両方を有する近赤外色素の開発に成功した。

研究成果の学術的意義や社会的意義

色素増感太陽電池(DSSC)のさらなる性能向上には、新たな近赤外光吸収色素の開発が必要不可欠である。DSSCでは、色素には光吸収帯域だけでなく、TiO₂との結合安定性および、TiO₂への電子注入性(光子収集性)が重要となっている。本研究では理論的・実験的アプローチの両面から、新規色素の開発を行い、これら課題を解決することに成功しており、効率的な新規材料開発への貢献が期待される。また、商業化のための安定した高効率DSSCの開発は、低環境負荷・低コストな太陽光エネルギー収穫の実現につながる。

研究成果の概要(英文)：Combined theoretical and experimental approaches have been implemented for the design and development of novel NIR dyes bearing various functional groups aiming towards improved NIR photoconversion and stability. A new method for the prediction of theoretical energy band diagram based on MO calculation was developed, which shows excellent match with the experimental energy band diagram counterparts. Our results have indicated that anchoring groups like phosphonic acid and cyanoacrylic acid exhibited opposite trends in terms of electron injection and their binding strength on TiO₂. Acrylic acid was found to be optimum anchoring group for both of the photon harvesting and binding stability. NIR dye with double anchoring groups (SQ-162) bearing both of the acrylic and phosphonic acids not only exhibited improved PCE but also about 550 times stronger binding on TiO₂ as compared to the dye SQ-140 bearing only cyanoacrylic acid.

研究分野：化学(複合化学)

キーワード：Structural optimization TD-DFT calculations Squaraine dyes Anchoring groups Binding stability DSSC

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1. 研究開始当初の背景

Techno-scientific developments on optimized and state-of-art dye-sensitized solar cells (DSSCs) is about the last two decades have witnessed the achievement of photoconversion efficiency (PCE) 12-14 %, nearly quantitative photon harvesting in visible wavelength region (400-750 nm). This offers an obvious hope for further enhancement in the PCE utilizing NIR/IR sensitizers since this region covers about 55 % of the photon flux of solar irradiation. At the same time, outdoor device stability >2.5 years suggests that there is a need for further enhancement in the device stability to compete with the commercial counterparts. Sensitizing dyes of DSSCs plays a pivotal role not only in being actual photon harvester but also their stability on mesoporous TiO₂ governs the device stability too. Dyes anchored on TiO₂ surface by most commonly used carboxylate or cyanoacrylate functional groups exhibited efficient electron injection but are desorbed from TiO₂ surface in the presence of humidity and high temperature, which is one of the serious obstacles towards the stability of DSSCs [1]. Using Azobenzene dyes has been shown that > 90 % of dye with -COOH anchoring group attached on TiO₂ surface get eliminated in 100 hours while > 80 % has remained after 2000 hours on the surface when put in water at 25°C for -Si(OEt)₃ anchoring group [2]. A sufficient coupling of electrons between the excited dye and TiO₂ has been the most accepted criteria for facile electron injection and photosensitization. The presence of sufficient electron density at LUMO of the dye ensures the good electronic coupling between the excited dye molecules and TiO₂, which ensures the facile electron injection. The applicant is involved in the design and development of NIR sensitizers for the last 10 years utilizing combined experimental and theoretical approaches. TD-DFT calculated results reveals that, unlike carboxylate and cyanoacrylate anchoring groups, there is no electron density at the anchoring group in the dye-containing -Si(OEt)₃. Report of very high photon harvesting in dyes with -Si(OEt)₃ despite lack of sufficient electron density at anchoring group laid the foundation for this proposal.

2. 研究の目的

The purpose of this proposal is to design novel NIR dyes aiming towards improved efficiency and stability of dye-sensitized solar cells and providing amicable solution utilizing combined theoretical and experimental approaches based on logical molecular design to address the following issues:

1. Proposal of the novel molecular structure for NIR dyes with high stability and efficient photosensitization.
2. Quantum chemical calculations to select the potential candidates and verify their usefulness by their synthesis, characterization, environmental stability and photosensitization.
3. To investigate the implication of molecular design on the differential photosensitization and proposal of optimum molecular framework having capability of improved stability and photoconversion efficiency.

3. 研究の方法

1. Gaussian program was used to assist the molecular design using a model unsymmetrical squaraine dye bearing different anchoring groups, which were subjected to structural optimization and calculation of electronic absorption spectra, energy of their HOMO and LUMO, energy band gap and finally theoretical energy band diagram taking TiO₂ as electron transporter and dye adsorption scaffold and most commonly used I⁻/I₃⁻ redox electrolyte. To make a balance between computation cost and accuracy, density functional theory (DFT) and TD-DFT under 6-311G basis, B3PW91 as functional, Polarization continuum solvent model using ethanol solvent as per the optimum calculation parameters based our previous results [3].

2. After the feedback from theoretical MO calculations, some of the potential candidate molecules were subjected to chemical synthesis and their photophysical characterizations. Experimental results were compared to theoretically calculated values to validate the calculated results along with the proposal of a novel dye molecular framework, which is expected to exhibit not only improved NIR photosensitization but also improved device stability after the DSSC fabrication.

3. Dye adsorption behaviour on the mesoporous TiO₂ was conducted by monitoring the rate of dye adsorption spectrophotometrically. At the same time, as an index of DSSC stability, dye binding strength was also estimated by measuring the total amount of adsorbed dye and estimating their rate of dye desorption from the TiO₂ surface after putting the dye-adsorbed TiO₂ in the acetonitrile-water mixture at room temperature for different time intervals followed by the estimation of the desorbed dye spectrophotometrically.

4. Some of the newly designed and potential NIR sensitizers were used for their relative photosensitization behaviour by DSSC fabrication utilizing TiO₂ for photoanode fabrication and most commonly employed I⁻/I₃⁻ redox electrolyte followed by evaluation of photovoltaic performance as well as device stability.

5. Finally, the implication of the nature of anchoring groups on their stability and photovoltaic performance. Such correlations are expected for the successful proposal of the optimum molecular structure of novel NIR dyes having good photon harvesting in the NIR region along with improved stability.

4. 研究成果

Theoretical MO Calculation

Along with enhancing the PCE, increasing the stability, is an important target that has to be achieved to accelerate the efforts of commercialization of DSSCs. The nature of anchoring groups present in the sensitizers not only control the PCE by controlling the efficiency of electron injection but also control the device stability by providing the binding strength. The high binding strength of the sensitizers along with the facile electron injection is highly desired for the fabrication of stable and efficient DSSCs. Taking this into consideration, a series of NIR dyes bearing the same π -molecular framework but different anchoring groups (SQ-138 to SQ-156) as shown in Figure 1 were designed and subjected to the quantum chemical calculations by Gaussian G09 aiming towards the investigation of their energetics, spectral behaviour and energy bandgap (E_g).

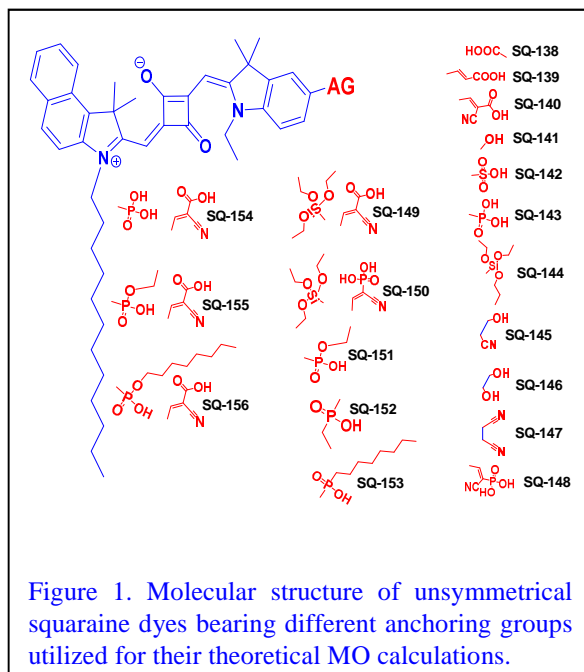


Figure 1. Molecular structure of unsymmetrical squaraine dyes bearing different anchoring groups utilized for their theoretical MO calculations.

Energetic cascade amongst the sensitizer, mesoporous TiO_2 and redox electrolyte is highly desired for the optimal functioning of the DSSCs. We have adopted a new method to construct the theoretical energy band diagram. Here HOMO energy level was calculated after structural optimization using 6-311G/DFT/B3PW91 and PCM model (Ethanol). Optimized structures were then used for TD/DFT excited state absorption spectral calculations and wave-length corresponding to the FWHM of the calculated spectrum was considered to be E_g followed by calculation of the energy of LUMO using the relation $\text{LUMO} = \text{HOMO} + E_g$.

A perusal of Figure 2, clearly corroborates that except two dyes that SQ-141 and SQ-146 bearing hydroxyl and catechol anchoring groups, all are suitable as sensitizers for the DSSCs using TiO_2 as an electron-acceptor scaffold and I^-/I_3^- redox electrolyte. In parallel to theoretical QC calculations, eight of the newly designed NIR dyes were also synthesized and subjected to their photophysical characterizations. Photophysical results for some of the experimentally synthesized dyes indicate only a difference of 60-70 nm (0.06 eV) in λ_{max} and (± 0.06 eV) in the E_g between the theoretical prediction and experiment results. At the same time, the experimental energy

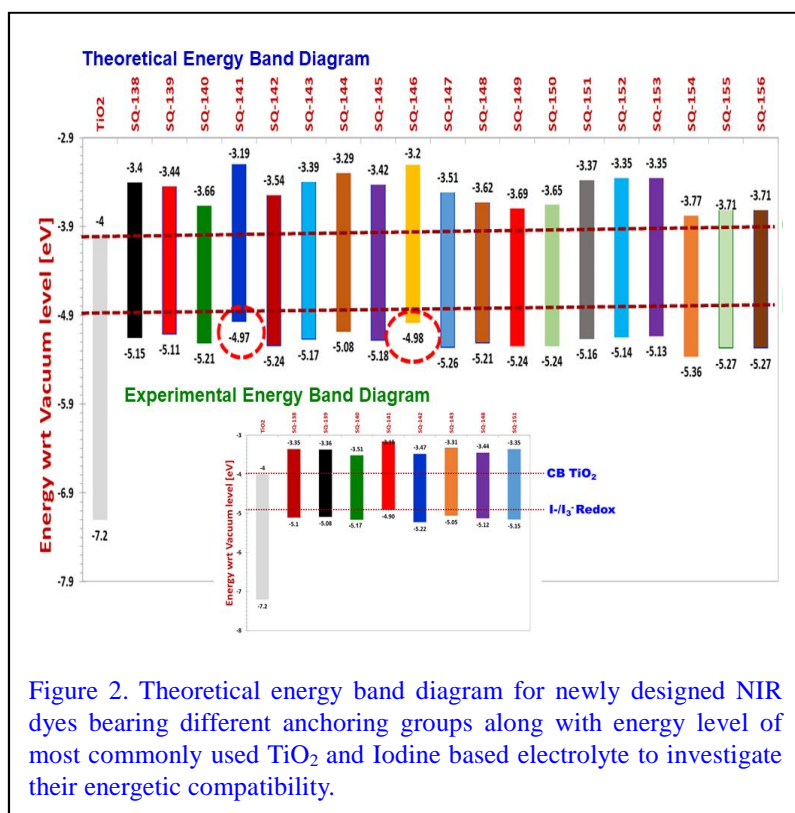


Figure 2. Theoretical energy band diagram for newly designed NIR dyes bearing different anchoring groups along with energy level of most commonly used TiO_2 and Iodine based electrolyte to investigate their energetic compatibility.

diagram for the synthesized dyes as shown in the inset of Figure 2, also exhibits an excellent match with the theoretically predicted results.

Synthesis and Photophysical Characterizations

After the feedback from theoretical MO calculations, 8 of the unsymmetrical squaraine (SQ) dyes such as SQ-138, SQ-139, SQ-140, SQ-141, SQ-142, SQ-143, SQ-148, SQ-151 bearing anchoring groups like carboxyl, acrylic acid, cyanoacrylic acid, hydroxyl, sulfonic acid, phosphonic acid, cyanophosphonic acid and Ethyl-cyanophosphonic acid, respectively, were first synthesized and their structural verification was

done by FAB-mass and NMR spectroscopy. After structural verification, they were subjected to optical characterizations by absorption and emission spectroscopy and electrochemical characterization by cyclic voltammetry (CV). An experimental energy band diagram for these dyes was constructed by estimating the HOMO from 1st oxidation potential of CV and E_g from the onset of optical absorption edge followed by calculation of LUMO energy using these parameters using the relation $LUMO = HOMO + E_g$.

Adsorption Behaviour and Binding Strength on Mesoporous TiO₂

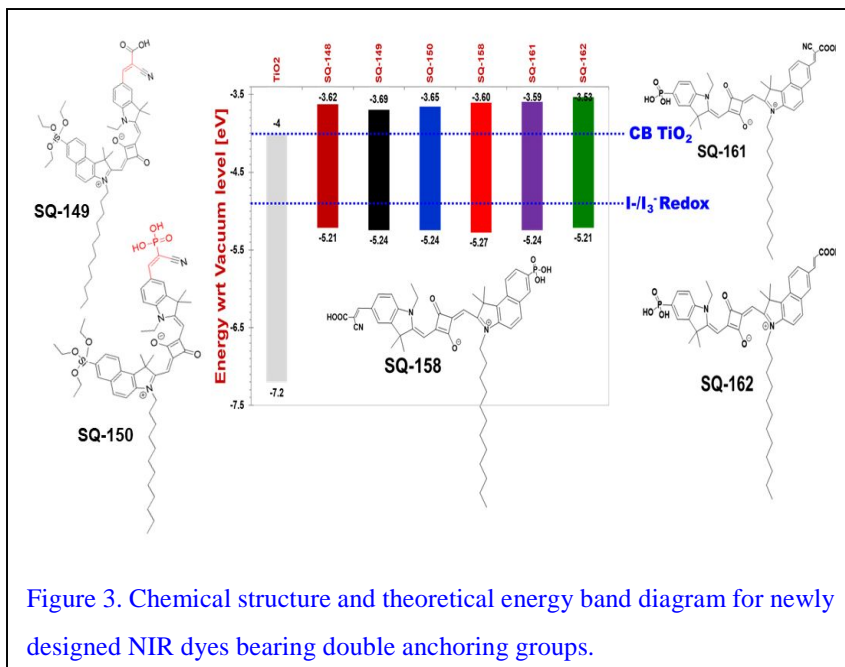
Control of dye adsorption on the TiO₂ surface plays a crucial role in controlling the PCE since a monolayer of dye is sufficient for optimal performance. Speedy dye adsorption on the wide bandgap semiconductor is highly desired to facilitate the production process of DSSCs industrially. Dyes like SQ-139, SQ-140, SQ-143, and SQ-148 bearing acrylic acid, cyanoacrylic acid, phosphonic acid, and cyano-phosphonic acid functional groups, respectively exhibited a faster rate of dye adsorption, which was attributed to the presence of multiple binding sites (plural -OH groups), multiple binding modes like mono, bi, and tridentate ligations (-OH groups) in the case of SQ-143 and SQ-148. At the same time, it is also controlled by enhanced activation of -OH groups on TiO₂ surface via protonation, and relatively lower value pK_a for carboxylic acid and phosphonic acids promote this activation. Anchoring groups not only control the PCE of DSSCs by controlling the efficiency of electron injection but also are responsible for the stability of the device by controlling the strength of bonding at the TiO₂ surface. The strength of binding of dyes on the TiO₂ surface is a very good indicator of the stability of DSSCs. Dyes with free phosphonic acid group exhibited remarkably high binding strength upon their adsorption on TiO₂ while Dye SQ-140 bearing cyanoacrylic acid anchoring group showed the weakest binding, where 99.8 % of dye leached out from TiO₂ surface in the solvent just only in 30 min. Introduction of the alkyl side chain in the phosphonate group (dyes SQ-151 and SQ-157) not only exhibited a hampered rate of dye adsorption but also with relatively weaker binding with TiO₂ due to the removal of >40 % of the dyes in the acetonitrile-water mixture at the room temperature. SQ-139 with acrylic acid although exhibited a little poor binding strength as compared to that of SQ-143 and SQ-148 bearing phosphonic and cyano phosphonic groups but exhibit about 14 times stronger binding than that of SQ-140 with cyanoacrylic acid.

DSSC Fabrication and Characterization

To investigate the influence of the nature of anchoring on photovoltaic behavior, some of the newly designed dyes were used as a sensitizer to fabricate the photoanode after their adsorption onto the mesoporous TiO₂. DSSCs were fabricated using dyes synthesized in this work keeping other variables such as dye concentration, the concentration of the CDCA, and redox electrolyte. Amongst various NIR sensitizers designed, SQ-140 exhibited the best photovoltaic performance with a PCE of 5.95%. This could be attributed to the good energetic matching and the highest diversion of the electron density clouds in LUMO (as indicated from QC calculations). Despite these merits in combination with swift dye adsorption, it suffers the problem of weak binding, which is not suitable for the realization of the stable DSSCs. Phosphonate-based anchoring group although exhibited very good and strong binding with TiO₂ but the relatively poor diversion of electron density at the anchoring group, and enhanced dye aggregation are bottlenecks of the facile electron injection leading to hampered photon harvesting. Although, alkyl substitution in phosphonate anchoring group (SQ-151 and SQ-157) resulted in suppressed dye aggregation leading to improved PCE supported by enhanced IPCE but their relatively slow rate of dye adsorption and hampered binding strength with TiO₂ poses a question mark on the implementation of this concept for design and development of novel NIR dyes with improved efficiency and stability. Unsymmetrical squaraine dye SQ-139 bearing acrylic acid seems to be a good balance in terms of the good electronic coupling with TiO₂ for facile electron injection leading to appreciable good PCE of 4.5 %, swift dye adsorption, and fairly good binding strength with TiO₂. Therefore, acrylic acid anchoring groups appears to be a good choice amongst the anchoring groups considering not only the photon harvesting but also the device stability.

Proposal of Novel NIR Dye Structure for Improved Stability and Efficiency

Results of the nature of anchoring groups on photon harvesting behaviour and binding strength on TiO₂ indicated that it is better to divide the role of imparting stability and photoconversion by incorporating dual anchoring groups. Acrylic and cyanoacrylic acid anchoring groups are good for photoconversion while phosphonic acid is good for strong binding. Silyl ester anchoring has already been reported to exhibit the strongest binding on the TiO₂ surface. Keeping these points into consideration novel NIR dyes with double anchoring groups with structure and theoretically calculated energy band diagram as shown in Fig. 3 were designed proposed aiming towards the design of novel NIR dyes with improved stability as well as PCE. It can be seen from this figure that all of the newly designed sensitizers are energetically matching for their compatibility with TiO₂ and iodine-based redox electrolyte for DSSC fabrication. QC calculation results have also indicated that there is sufficient diversion of electron density on cyano-acrylic and acrylic acid



SQ-148 bearing free Phosphonic acids (0.9 %) and only slightly lower than SQ-139 bearing single acrylic acid (4.5 %). Therefore, the design of SQ-162 offers good hope for the further refinement of the molecular structure utilizing the main molecular framework with extended π -conjugation for the design of novel NIR dyes with further improvement in PCE while maintaining the stronger binding strength with TiO_2 leading stable and efficient DSSCs.

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anchoring groups ensuring the facile electron injection. One of the proposed dyes, SQ-162 bearing phosphonic and acrylic acid anchoring group was synthesized, and used for photophysical investigations and DSSC fabrication. SQ-162 with double anchoring group exhibited extremely high binding with TiO_2 , which is >550 times stronger than the cyano acrylic anchoring group. At the same time, the observed PCE of about 2.9 % is much improved comparing

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〔図書〕 計0件

〔産業財産権〕

〔その他〕

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6. 研究組織

	氏名 (ローマ字氏名) (研究者番号)	所属研究機関・部局・職 (機関番号)	備考
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7. 科研費を使用して開催した国際研究集会

〔国際研究集会〕 計0件

8 . 本研究に関連して実施した国際共同研究の実施状況

共同研究相手国	相手方研究機関
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