

化學系50周年  
慶祝大會

慶祝輔大化學系五十週年慶

## 應用合成肽和分子印模對氣味篩選之研究

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輔仁大學 化學系





# 慶祝輔大化學系五十週年慶





on Ag(111): The Catalytic Role of H<sub>2</sub>O  
"Water Molecules" and "High Pressure"  
Department of Chemistry, Tsinghua University

清华大学化学系第十周年纪念













廖祥

超分子

Organic  
constructed  
Acid with  
channels.

Yun Pan,  
Feng  
University,  
J. Liu



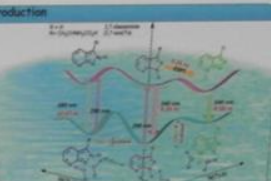
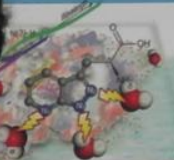
# Probing Water Microsolvation Dynamics of Heme proteins toward Photochemical Application

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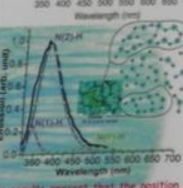
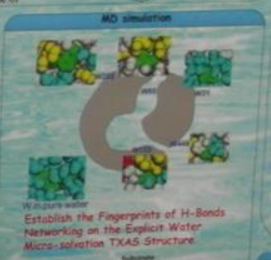
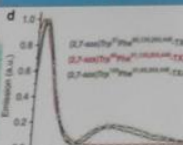
## Abstract

Scientists have made tremendous endeavors in attempts to gain understanding of the water molecules in proteins via indirect measures, such as molecular simulation and/or probing the polarity of the local environment. Probing the water environment of a specifically interesting site in proteins thus may provide understanding the underlying mechanism. Unfortunately, although enormous efforts have been made in the characterization of fundamental aqueous phenomena on protein surfaces, little insight has been gained into water micro-solvation in protein. The newly-developed tryptophan analogue, (2,7-aza)Trp, whose water catalyzed proton transfer properties. The resulting multiple emissions provide unique fingerprints that can be exploited for directly sensing the water environment in a protein. Here we selected the structurally pending thromboxane  $A_2$  synthase (TXAS), an endoplasmic reticulum membrane protein with multiple tryptophans, as a prototype to demonstrate the feasibility of (2,7-aza)Trp in probing water environments. The incorporation of (2,7-aza)Trp as a novel optical probe that allows transmission of its surrounding water environment into unique fluorescence spectral features. In combination with MD simulation, future quantitative correlation for the ESPT dynamics versus number/orientation of water molecules is feasible, showing different correlation between the substrate access channel, aqueduct water channel, and protein surface in, e.g., TXAS. The superb water sensing capability in terms of the N<sub>1</sub>-HN<sub>2</sub>-H equilibrium that provides an unprecedented tool for probing the water environment in bio-systems on a structural basis.

## Introduction



## Characteristics of the Trp Analogue Probing Water



The results present that the position W65 is subject to a Water-deficient microenvironment wherein the lack of surrounding water molecules

## Water shell



## Summary

(2,7-aza)Trp mutant maintains its parent wild-type TXAS structure. Exploiting co-translational (2,7-aza)Trp as a novel optical probe that allows transmission of its surrounding water environment into unique fluorescence spectral features. In combination with MD simulation, future quantitative correlation for the ESPT dynamics versus number/orientation of water molecules is feasible, showing different correlation between the substrate access channel, aqueduct water channel and protein surface in, e.g., TXAS. The superb water sensing capability in terms of the N<sub>1</sub>-HN<sub>2</sub>-H equilibrium thus provides an unprecedented tool for probing the water environment in bio-systems on a structural basis.

Supporting Information: Supporting Information for this article is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jchemeduc.1c00000.









游源祥

# Fabrication and characterization of poly (vinyl alcohol)/functionalized graphene oxide nanofibers produced by electrospinning method

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**Abstract:**  
A series of poly (vinyl alcohol) (PVA)/functionalized graphene oxide (FGO) nanofibers with low loading ratios of FGO to PVA were fabricated by electrospinning. The prepared PVA/FGO nanocomposites were dispersed in water phase followed by electrospinning treatment under different operational parameters (i.e., applied voltage and FGO content) to give nanofibers of various diameters and morphologies. The morphology, diameter and structure of electrospun nanofibers and FGO were characterized by Fourier transform infrared (FTIR) spectroscopy, X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), transmission electron microscopy (TEM), SEM image showed that the morphologies of the nanofibers were improved by the incorporation of FGO at a low loading content (e.g., 0.1–0.5 wt %). The crystallinity, storage modulus and thermal stability of PVA/FGO nanofibers were also studied.

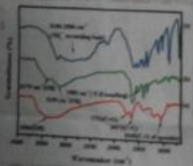
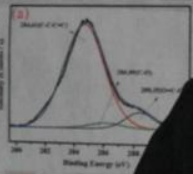
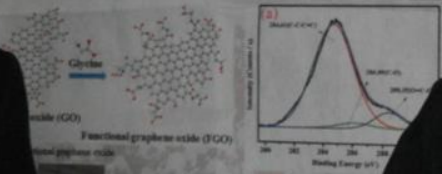


Figure 2. FTIR spectra of (a) graphene oxide (b) FGO (c) PVA/FGO nanofibers.

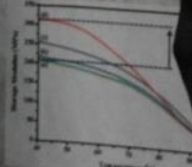


Figure 3. DSC curves with different ratios of FGO in the FGO/PVA nanocomposites: (a) pure PVA, (b) 0.1% FGO/PVA, (c) 0.3% FGO/PVA, (d) 0.5% FGO/PVA.

### Conclusions:

A series of FGO/PVA nanocomposites were prepared successfully and characterized by scanning electron microscopy analysis. A low loading ratio of FGO could improve the morphology and dispersibility of FGO in the electrospinning. In this study, the morphology and properties of PVA/graphene oxide nanofibers were also studied.

### Acknowledgement

This research was supported by the Ministry of Science and Technology, Taiwan, R.O.C.







































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慶祝輔大化學系五十





五十週年慶





# 南大化學系五十週年





# 大化學系五十週年慶





















































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輔大化學系二十週年

陳元璋 教授



















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