



## Dr. Vignesh Kumaravel

Senior Research Scientist,  
Innovation center,  
Institute of Technology Sligo, Ireland

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Google Scholar Citations: 1535

h-index: 24

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Specialization: Materials for Energy, Environment and Health

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### ACADEMIC APPOINTMENTS

#### Senior Scientist

(From March 2018- to date)

EU funded Renewable Engine project at **Institute of Technology Sligo, Ireland**. I am supervising Ph.D student's research work and involving in the fabrication of nanomaterials for antimicrobial indoor building materials, CO<sub>2</sub> conversion into fuels, thermally stable energy storage devices, hydrogen production from wastewater, 2D membranes for water treatment *via* a sustainable technology.

#### Assistant Research Scientist

(October 2016 to January 2018)

Department of Chemical engineering, **Texas A & M University at Qatar**. I supervised the undergraduate and master student's research projects. I am also involved in the fabrication of photocatalysts for hydrogen production using seawater and wastewater.

#### Post-Doctoral Researcher

(April 2015 – May 2016)

School of Materials and Mineral Resources Engineering, **Universiti Sains Malaysia**. I supervised the research projects for master's and Ph.D. students. During the same period, I worked as an R & D manager in *Anano Sphere Sdn Bhd*, Malaysia (producing the photocatalyst liquid spray to purify indoor air).

#### Assistant Professor

(March 2014 – February 2015)

Department of Inorganic Chemistry, **Yeungnam University, Republic of Korea**. I conducted the course work (renewable energy) for master's and Ph.D. students. I also carried out my research in photocatalysis for water treatment.

#### Assistant Professor

(January 2013 – February 2014)

**C. P. A. College, Tamilnadu, India**. I conducted the coursework and practical classes of MSc Chemistry and Industrial Chemistry students. Eight MSc and four MPhil chemistry students completed their research projects under my guidance.

#### Research Fellow/Guest Lecturer

(June 2009 – December 2012)

I have worked in the UGC sponsored major research project in **Thiagarajar College, Tamilnadu, India**. I have also completed my Ph.D (Photocatalytic activity of surface modified semiconductor nanoparticles for environmental remediation) during the same period from Madurai Kamaraj University, India. In addition, six MPhil students completed their research project under my co-

guidance. I also worked as a guest lecturer to conduct the course work for MSc and practical classes for the BSc students.

### **Lecturer**

**(July 2008- May 2009)**

Department of Chemistry, **Sri Kaliswari College, Tamilnadu, India**. I conducted the practical classes and course work for MSc and BSc students. Two MSc students completed their research projects under my guidance.

### **INDUSTRIAL EXPERIENCE**

#### **R & D Manager**

**(April 2015 – May 2016)**

R & D manager in the quality control at **Anano Sphere Sdn Bhd**, Malaysia to produce photocatalyst liquid spray to purify indoor air and the disinfection of microbes.

#### **Project Assistant**

**(Dec 2007 - March 2008)**

Organic synthesis laboratory, **Syngene International Ltd, Bangalore, India**. I was involved in the synthesis of pyrimidine compounds for biological activity.

### **RESEARCH INTERESTS**

#### ***10 Years of Research Experience in Materials Science***

**Thermally stable battery/supercapacitors for Electric Vehicles, CO<sub>2</sub> conversion into C1 and C2 fuels, Electro-catalysts for energy production, CO<sub>2</sub> capture, Hydrogen production from seawater/wastewater splitting, Antimicrobial polymers for food packaging polymers and biomedical implants, Hydrophobic coatings/self-cleaning from agriculture waste, 2D membranes for the disinfection of microbes.**

In this present scenario, global warming, water scarcity, infectious diseases, and energy crisis are serious problems to humanity. The nanomaterials developed in my research work are successfully addressing those issues in a sustainable way. Furthermore, the materials and technology developed in my research promote the national and international research collaborations.



### **TEACHING EXPERIENCE**

#### ***5+ Years of Teaching Experience***

**Five years of teaching experience** in various fields such as Industrial Chemistry, Analytical chemistry, Environmental Chemistry, Water treatment, Nano-chemistry, Organic Chemistry, Inorganic Chemistry, Pharmaceutical Chemistry, etc.) **in India, and Republic of Korea**. For more insight on the didactic skills please refer my lecture published in the YouTube <https://www.youtube.com/watch?v=2oauUVpQc7k> which was given for the Ph.D students at the 3<sup>rd</sup> European summer school on advanced oxidation process at Spain during June 2019.

### ACADEMIC DEGREES

- 2013 - Doctor of Philosophy (Ph. D) Chemistry** - Madurai Kamaraj University, India  
**Highly Commended**
- 2008 - Master of Science (MSc) Pharmaceutical Chemistry**, Madurai Kamaraj University, India  
**72.20 % - First Rank with Gold Medal**
- 2007 - Certificate in Industrial Safety**, Madurai Kamaraj University, India  
**First Class**
- 2006 - Bachelor of Science (BSc) Chemistry**, Manonmaniam Sundaranar University, India  
**81.5 % - First Class with Distinction**

### PUBLIC PROFESSIONAL ACTIVITIES

**Guest Editor – Catalysts**

[https://www.mdpi.com/journal/catalysts/special\\_issues/Electrocatalysis\\_Electrode\\_Energy](https://www.mdpi.com/journal/catalysts/special_issues/Electrocatalysis_Electrode_Energy)

*Issues - Photocatalytic Hydrogen Evolution*

*Electrocatalysis and Electrode Materials for Energy Production*

**Research proposals Examiner** for funding agencies in Chile (Chilean National Science and Technology Commission), and Poland (National Science Centre).

**Committee member** of Research and Innovation of Institute of Technology Sligo, Ireland

**Reviewer** for various Elsevier, ACS, Wiley, and RSC Journals. Reviewed more than 50 research articles.

**Ph.D Dissertation Examiner** for Madurai Kamaraj University, Bharathiar University, and Anna University, India.

### MEMBERSHIP IN PROFESSIONAL SOCIETIES

American Ceramic Society, European Microscopy Society, Irish Catalysis Society

### RESEARCH PROJECTS SUPERVISION

**Completed Master of Science theses – 10**

**Completed Master of Philosophy theses – 10**

**PhD theses in progress - 2** (Co-Supervisor at IT Sligo, Ireland)

### RESEARCH GRANTS AWARDED

**Role:** Co-investigator

**Funding Agency:** TRGS, Malaysia

**Project Title:** Nanocatalyst Inspired antimicrobial polypropylene nanocomposite for biomedical applications

**Period:** 02/12/2016 to 01/11/2019

**Amount:** USD 177,469

**Role:** Co-investigator

**Funding Agency:** FRGS, Malaysia

**Project Title:** Investigation on the durability, growth mechanism and bonding interactions of superhydrophobic surfaces made from waste materials

**Period:** 02/11/2015 to 01/11/2017

**Amount:** USD 30,548

**Role:** Co-investigator

**Funding Agency:** RUI, Malaysia

**Project Title:** Development of g-C<sub>3</sub>N<sub>4</sub> Supported ZnO Nanotriangles for Super Hydrophobic Self Cleaning Applications

**Period:** 01/03/2016 to 28/02/2018

**Amount:** USD 23,108

**Role:** Principal Investigator

**Funding Agency:** Institute of Technology Sligo- Capacity Building Grant

**Project Title:** Photoelectrochemical conversion of carbon dioxide into fuels

**Period:** Dec 2019 to Nov. 2020

**Amount:** EUR 18,000

**Role:** Principal Investigator

**Funding Agency:** Institute of Technology Sligo- Capacity Building Grant

**Project Title:** Thermally stable energy storage devices

**Period:** March 2021 to Feb 2022

**Amount:** EUR 23,000

### LIST OF PUBLICATIONS (\* *Corresponding author*)

#### Peer-reviewed International Journal Papers (SCI/Scopus)

#### 2021

1. V. Kumaravel \*, J. Bartlett, S. C. Pillai, Solid electrolytes for high-temperature stable batteries and supercapacitors, **Advanced Energy Materials** 11 (2021) 2002869
2. K. M. Nair, V. Kumaravel, S. C. Pillai, Carbonaceous cathode materials for electron-Fenton technology: Mechanism, Kinetics, Recent Advances, Opportunities and Challenges, **Chemosphere** 269 (2021) 129325
3. V. Kumaravel \*, K. M. Nair, S. Mathew, J. Bartlett, S. C. Pillai, Antimicrobial TiO<sub>2</sub> nanocomposite coatings for surfaces, and medical implants, **Chemical Engineering Journal** (2021) 129071.
4. S. Mathew, P. Ganguly, K. M. Nair, K. O' Dowd, S. Dervin, V. Kumaravel \*, D. D. Dionysiou, S. C. Pillai, 2D Materials: Membranes for water treatment, fuel cells and batteries, **ACS ES&T Engineering** (Under Submission)

#### 2020

5. V. Kumaravel \*, J. Bartlett, S. C. Pillai, Photoelectrochemical conversion of carbon dioxide (CO<sub>2</sub>) into fuels and value-added products, **ACS Energy Letters** 5 (2020) 486-519.
6. V. Kumaravel \*, S. Rhatigan, S. Mathew, M. Michel, J. Bartlett, M. Nolan, S.J. Hinder, A. Gasco, C. Ruiz-Palomar, D. Hermosilla, S. C. Pillai, Mo doped TiO<sub>2</sub>: impact on oxygen vacancies, anatase phase stability and photocatalytic activity, **Journal of Physics: Materials** 3, (2020) 025008.
7. CC Farrell, Al Osman, R Doherty, M Saad, X Zhang, A Murphy, J Harrison, ASM Vennard, V. Kumaravel, AH Al-Muhtaseb, DW Rooney, Technical challenges and opportunities in realising a circular economy for waste photovoltaic modules, **Renewable and Sustainable Energy Reviews**

128 (2020) 109911.

8. N. Sutanto, K.A. Saharudin, S. Sreekantan, **V. Kumaravel** \*, H.M. Akil, Heterojunction catalysts  $gC_3N_4/3ZnO-c-Zn_2Ti_3O_8$  with highly enhanced visible-light-driven photocatalytic activity, **Journal of Sol-Gel Science and Technology** 93 (2020) 354-370.
9. J.Y. Do, N. Son, R.K. Chava, K.K. Mandari, S. Pandey, **V. Kumaravel**, T. S. Senthil, S. Woo Joo, M. Kang, Plasmon-Induced Hot Electron Amplification and Effective Charge Separation by Au Nanoparticles Sandwiched between Copper Titanium Phosphate Nanosheets and Improved Carbon Dioxide Conversion to Methane, **ACS Sustainable Chemistry and Engineering**, 8 (2020) 18646-18660.
10. S. Mathew, P. Ganguly, **V. Kumaravel**, J. Harrison, S. J Hinder, J. Bartlett, S. C. Pillai, Effect of chalcogens (S, Se, and Te) on the anatase phase stability and photocatalytic antimicrobial activity of  $TiO_2$ , **Materials Today: Proceedings** 33 (2020) 2458-2464.
11. S. Sundararaju, A. Manjula, **V. Kumaravel**, T. Muneeswaran, T. Vennila, Biosorption of nickel ions using fungal biomass *Penicillium* sp. MRF1 for the treatment of nickel electroplating industrial effluent, **Biomass Conversion and Biorefinery** (2020)
12. P. Forouzandeh, **V. Kumaravel**, S. C Pillai, Electrode Materials for Supercapacitors: A Review of Recent Advances, **Catalysts** 10 (2020) 969

## 2019

13. **V. Kumaravel** \*, S. Rhatigan, S. Mathew, J. Bartlett, M. Nolan, S.J. Hinder, P.K. Sharma, A. Singh, J.A. Byrne, J. Harrison, S. C. Pillai, Indium doped  $TiO_2$  photocatalysts with high temperature anatase stability, **Journal of Physical Chemistry C** 123 (2019) 21083-21096.
14. **V. Kumaravel** \*, S. Mathew, J. Bartlett, S. C. Pillai, Photocatalytic hydrogen production using metal doped  $TiO_2$ : A review of recent advances, **Applied Catalysis B: Environmental** 244 (2019) 1021-1064
15. Sriharan N, Senthil TS, **V. Kumaravel** \*, Fabrication of hydrophobic coatings using sugarcane bagasse waste ash as silica source, **Applied Sciences** 9 (2019) 190
16. **V. Kumaravel** \*, M. D. Imam, A. Badreldin, R. K. Chava, J. Y. Do, M. Kang, A. Abdel-Wahab, Photocatalytic Hydrogen Production: Role of Sacrificial Reagents on the Activity of Oxide, Carbon, and Sulfide Catalysts, **Catalysts** 2019, 9, 276
17. N. Basiron, S. Sreekantan, H. Md Akil, K. A. Saharudin, N. H. Harun, R. Basria SMN Mydin, A. Seenii, N. R. Abdul Rahman, F. Adam, A. Iqbal, **V. Kumaravel**, Effect of  $Li-TiO_2$  nanoparticles incorporation in LDPE polymer nanocomposites for biocidal activity, **Nano-Structures and Nano-Objects** 19 (2019) 100359

## 2018

18. **V. Kumaravel** \*, A. Abdel-Wahab, A Short Review on Hydrogen, Biofuel, and Electricity Production Using Seawater as a Medium, **Energy & Fuels** 32 (2018) 6423–6437
19. S. Mathew, P. Ganguly, S. Rhatigan, **V. Kumaravel**, C. Byrne, S. Hinder, J. Bartlett, M. Nolan, S. Pillai, Cu-Doped  $TiO_2$ : Visible Light Assisted Photocatalytic Antimicrobial Activity, **Applied Sciences** 8 (2018) 2067.
20. K. Saharudin, S. Sreekantan, N. Basiron, Y. Khor, N. Harun, R. SMN Mydin, H. Md Akil, A.Seeni, **K. Vignesh**, Bacteriostatic Activity of LLDPE Nanocomposite Embedded with Sol–Gel Synthesized  $TiO_2/ZnO$  Coupled Oxides at Various Ratios, **Polymers** 10 (2018) 878
21. S. Rajamohan, **V. Kumaravel** \*, A. Abdel-Wahab, R. Muthuramalingam, S. Ayyadurai, Exploration of Ag decoration and Bi doping on the photocatalytic activity  $\alpha-Fe_2O_3$  under simulated solar light irradiation, **The Canadian Journal of Chemical Engineering** 96 (2018) 1713-1722
22. K. A. Saharudin, S. Sreekantan, N. Basiron, K. C. Lee, **V. Kumaravel** \*, T. T. Abdullah, Z.

A. Ahmad, Improved super-hydrophobicity of eco-friendly coating from palm oil fuel ash (POFA) waste, **Surface and Coatings Technology** 337 (2018) 126-135

23. N. Basiron, S. Sreekantan, K. A. Saharudin, Z. A. Ahmad, **V. Kumaravel** \*, Improved Adhesion of Nonfluorinated ZnO Nanotriangle Superhydrophobic Layer on Glass Surface by Spray-Coating Method, **Journal of Nanomaterials** (2018) Article ID 7824827

24. S. Sreekantan, K. A. Saharudin, N. Basiron, R. Basria SMN Mydin, O. C. Teng, **V. Kumaravel**, Phosphorus and Carbon Co-Doped TiO<sub>2</sub> Nanotube Arrays for Excellent ROS Production, **Reactive Oxygen Species** 6 (2018) 17.

## 2017

25. S. Rajamohan, **V. Kumaravel** \*, R. Muthuramalingam, S. Ayyadurai, A. Abdel-Wahab, B. S. Kwak, M. Kang, S. Sreekantan, Fe<sub>3</sub>O<sub>4</sub>-Ag<sub>2</sub>WO<sub>4</sub>: Facile synthesis, characterization and visible light assisted photocatalytic activity, **New Journal of Chemistry** 41 (2017) 11722-11730

## 2016

26. N. N. Hlaing, **K. Vignesh**\*, S. Sreekantan, S.-Y. Pung, H. Hinode W. Kurniawan, R. Othman, A.A. Thant, A. R. Mohamed, C. Salim, Effect of cetyl trimethyl ammonium bromide concentration on structure, morphology and carbon dioxide adsorption capacity of calcium hydroxide-based sorbents, **Applied Surface Science** 363 (2016) 586–5922.

27. F. D. M. Daud, **K. Vignesh**\*, S. Sreekantan, A. R. Mohamed, M. Kang, B. S. Kwak, Ca(OH)<sub>2</sub> nano-pods: investigation on the effect of solvent ratio on morphology and CO<sub>2</sub> adsorption Capacity, **RSC Advances** 6 (2016) 36031–36038.

28. F. D. M. Daud, **K. Vignesh**\*, S. Sreekantan, A. R. Mohamed, Improved CO<sub>2</sub> adsorption capacity and cyclic stability of CaO sorbents incorporated with MgO, **New Journal of Chemistry** 40 (2016) 231-237.

29. R. Satheesh, **K. Vignesh**, M. Rajarajan, A. Suganthi, S. Sreekantan, M. Kang, B. S. Kwak, Removal of congo red from water using quercetin modified α-Fe<sub>2</sub>O<sub>3</sub> nanoparticles as effective nanoadsorbent, **Materials Chemistry and Physics** 180 (2016) 53-65.

## 2015

30. **K. Vignesh**\*, M. Kang, Facile synthesis, characterization and recyclable photocatalytic activity of Ag<sub>2</sub>WO<sub>4</sub>@g-C<sub>3</sub>N<sub>4</sub>, **Materials Science and Engineering B** 199 (2015) 30–36.

31. **K. Vignesh**\*, S. Kang, B.S. Kwak, M. Kang, Facile synthesis of meso-porous ZnO nanotriangular prisms with enhanced photocatalytic activity, **RSC Advances** 5 (2015) 30120–30124.

32. **K. Vignesh**\*, S. Kang, B.S. Kwak, M. Kang, Meso-porous ZnO nano-triangles @ graphitic-C<sub>3</sub>N<sub>4</sub> nano-foils: Fabrication and Recyclable photocatalytic activity, **Separation and Purification Technology** 147 (2015) 257–265.

33. **K. Vignesh**\*, A. Suganthi, B.-K. Min, M. Kang, Fabrication of meso-porous BiOI sensitized zirconia nanoparticles with enhanced photocatalytic activity under simulated solar light irradiation, **Applied surface Science** 324 (2015) 652-661.

34. **K. Vignesh**\*, A. Suganthi, B.-K. Min, M. Rajarajan, M. Kang, Designing of YVO<sub>4</sub> supported β-Agl nano-photocatalyst with improved stability, **RSC advances** 5 (2015) 576-585.

35. B.S. Kwak, **K. Vignesh**, N.-K. Park, H. Ryu, J.-I. Baek, M. Kang, Methane formation from photoreduction of CO<sub>2</sub> with water using TiO<sub>2</sub> including Ni ingredient, **Fuel** 143 (2015) 570-576.

## 2014

36. **K. Vignesh** \*, A. Suganthi, B.-K. Min, M. Kang, Photocatalytic activity of magnetically

recoverable  $\text{MnFe}_2\text{O}_4/\text{g-C}_3\text{N}_4/\text{TiO}_2$  nanocomposite under simulated solar light irradiation, **Journal of Molecular Catalysis A: Chemical** 395 (2014) 373–383.

37. R. Satheesh, K. Vignesh, A. Suganthi, M. Rajarajan, Visible light responsive photocatalytic applications of transition metal ( $\text{M} = \text{Cu}, \text{Ni}$  and  $\text{Co}$ ) doped  $\text{Fe}_2\text{O}_3$  nanoparticles, **Journal of Environmental Chemical Engineering** 2 (2014) 1956–1968.

38. K. Vignesh, R. Priyanka, R. Hariharan, M. Rajarajan, A. Suganthi, Fabrication of  $\text{CdS}$  and  $\text{CuWO}_4$  modified  $\text{TiO}_2$  nanoparticles and its photocatalytic activity under visible light irradiation, **Journal of industrial and engineering chemistry** 20 (2014) 435–443.

39. K. Vignesh, M. Rajarajan, A. Suganthi, Visible light assisted photocatalytic performance of  $\text{Ni}$  and  $\text{Th}$  co-doped  $\text{ZnO}$  nanoparticles for the degradation of methylene blue dye, **Journal of industrial and engineering chemistry** 20 (2014) 3826–3833.

40. K. Vignesh \*, M. Rajarajan, A. Suganthi, Photocatalytic degradation of erythromycin under visible light by zinc phthalocyanine-modified titania nanoparticles, **Materials Science in Semiconductor Processing** 23 (2014) 98–103.

41. P. Malathy, K. Vignesh, M. Rajarajan, A. Suganthi, Enhanced photocatalytic performance of transition metal doped  $\text{Bi}_2\text{O}_3$  nanoparticles under visible light irradiation, **Ceramics International** 40 (2014) 101–107.

## 2013

42. K. Vignesh, R. Hariharan, M. Rajarajan, A. Suganthi, Photocatalytic performance of  $\text{Ag}$  doped  $\text{SnO}_2$  nanoparticles modified with curcumin, **Solid State Sciences** 21 (2013) 91–99.

43. K. Vignesh, R. Hariharan, M. Rajarajan, A. Suganthi, Visible light assisted photocatalytic activity of  $\text{TiO}_2$ -Metal vanadate ( $\text{M} = \text{Sr}, \text{Ag}$  and  $\text{Cd}$ ) nanocomposites, **Materials science in Semiconductor Processing** 16 (2013) 1521–1530.

44. K. Vignesh, R. Priyanka, M. Rajarajan, A. Suganthi, Photoreduction of  $\text{Cr(VI)}$  in water using  $\text{Bi}_2\text{O}_3$ - $\text{ZrO}_2$  nanocomposite under visible light irradiation, **Materials Science and Engineering B** 178 (2013) 149–157.

## 2012

45. K. Vignesh, A. Suganthi, M. Rajarajan, R. Sakthivadivel, Visible light assisted Photodecolorization of eosin-Y in aqueous solution using hesperidin modified  $\text{TiO}_2$  nanoparticles, **Applied Surface Science** 258 (2012) 4592–4600.

46. K. Vignesh, A. Suganthi, M. Rajarajan, S.A. Sara, Photocatalytic activity of  $\text{AgI}$  sensitized  $\text{ZnO}$  nanoparticles, **Powder Technology** 224 (2012) 331–337.

## Chapters in International books

47. A. J. Nathanael, K. Kannaiyan, A.K. Kunhiraman, V. Kumaravel \*, Nanomaterials for detection and removal of gases, **Nanomaterials for Sustainable Energy and Environmental Remediation**, Elsevier 2020, 219–260

48. S. Mathew, P. Ganguly, V. Kumaravel, J. Bartlett, S. C. Pillai, Solar light-induced photocatalytic degradation of pharmaceuticals in wastewater treatment, **Nano-Materials as Photocatalysts for Degradation of Environmental Pollutants**, Elsevier 2020, 219–260

49. K. M. Nair, P. Ganguly, S. Mathew, V. Kumaravel, S. C. Pillai,  $\text{TiO}_2$  based Z-scheme photocatalysts for energy and environmental application, **Heterostructured photocatalysts for solar energy**, Elsevier 2020, 257–282.

50. V. Kumaravel \*, S. Somasundaram, Exploitation of Nanoparticles as Photocatalysts for Clean and Environmental Applications, **Advanced Nanostructured Materials for Environmental Remediation**, Springer Cham 2019, 279–319.

51. S. Somasundaram, V. **Kumaravel** \*, Application of Nanoparticles for Self-Cleaning Surfaces, ***Emerging Nanostructured Materials for Energy and Environmental Science***, Springer Cham 2019, 471-498.
52. K. Kannaiyan, R. Sadr, V. **Kumaravel**, Application of Nanoparticles in Clean Fuels, ***Nanostructured Materials for Energy Related Applications***, Springer Cham 2019, 223-242.
53. S. Somasundaram, P. Veerakumar, K.-C. Lin, V. **Kumaravel** \*, Application of Nanocomposites for Photocatalytic Removal of Dye Contaminants, ***Photocatalytic Functional Materials for Environmental Remediation***, John Wiley & Sons, Inc. 2019, 131-161.
54. A. J. Nathanael, T. H. Oh, V. **Kumaravel** \*, Designing Smart Nanotherapeutics, ***Toxicity of Nanomaterials Environmental and Healthcare Applications***, CRC Press, 2019.

#### International Book Publication:

**Status:** On-going

**Publication Date:** July 2021

**Authors:** Vignesh Kumaravel, Suresh Pillai – IT Sligo, Ireland

**Book Title:** Insights of Photocatalysis

**Publisher:** De Gruyter

#### INTERNATIONAL and NATIONAL CONFERENCES

S. No	Date	Particulars	Venue
1	February 2010	RSC, CRSI sponsored “4 <sup>th</sup> CRSI-RSC National Symposium in Chemistry”	Indian Institute of Chemical Technology, Hyderabad, India
2	September 2010	UGC, CSIR, DRDO sponsored National seminar on “Emerging Trends in Chemistry”	C.P.A. College, Bodinayakanur, Tamilnadu, India
3	March 2011	CSIR, UGC and DST sponsored National Seminar on “Nanostructured Materials and Applications”	Madurai Kamaraj University, Madurai, Tamilnadu, India
4	August 2011	Third International Conference on Frontiers in Nanoscience and Technology, Cochin Nano- 2011”	Cochin University of Science and Technology, Cochin, Kerala, India
5	December 2011	International Conference on Nanomaterials and Nanotechnology-ICNANO-2011	University of Delhi, New Delhi, India

6	February 2012	14 <sup>th</sup> CRSI National Symposium in Chemistry	NIIST, Thiruvananthapuram, Kerala, India.
7	October 2012	National Seminar on Emerging Trends in Chemistry (ETC-4)	C.P.A. College, Bodinayakanur, Tamilnadu, India
8	October 2012	Second International conference on Advanced Oxidation processes	Mahatma Gandhi University, Kottayam, India
9	December 2012	International conference on Frontiers in Nanotechnology (5 <sup>th</sup> Bangalore Nano)	The Lalit Ashok, Bangalore (organized by Jawaharlal Nehru center for Advanced Research (JNCASR), Bangalore), India
10	July 2012	International conference on Nanoscience + Nanotechnology	Sorbone University, Paris, France
11	May 2014	2 <sup>nd</sup> USA International Conference on Surfaces, Coatings and Nanostructured Materials (NANOSMAT-USA)	Rice University, Houston, Texas, USA
12	November 2014	Korean Society of Industrial and Engineering Chemistry (KSIEC) Fall meeting	Daegu, Republic of Korea
13	Feb 2014	National Conference on Advanced Materials: Processing and Characterization	National Institute of Technology. Tiruchirappalli, India
14	July 2015	International Conference on Sustainable Materials Science and Technology	Paris, France
15	April 2019	Environ conference: 29 <sup>th</sup> Irish Environmental Researchers Colloquium	IT Carlow, Ireland
16	July 2019	2nd Global Forum on Advanced Materials and Technologies for Sustainable Development (GFMAT-2) and 4th International Conference on Innovations in Biomaterials, Biomanufacturing, and Biotechnologies (Bio-4)	Toronto, Canada

#### Invited Talks as Keynote Speaker:

- ***Metal oxide Nanocomposites: Antimicrobial food packaging and biomedical polymers*** – 3<sup>rd</sup> BK21 + International Symposium on photo-biochemistry in Yeungnam University, Republic of Korea on January 10<sup>th</sup>, 2020.
- ***High temperature stable titania for indoor antimicrobial coatings*** - 2<sup>nd</sup> BK21 + International Symposium on photo-biochemistry in Yeungnam University, Republic of Korea on January 11<sup>th</sup>, 2019.
- ***Photocatalysis of Nanocomposites towards environmental sustainability*** - 1<sup>st</sup> BK21 + International Symposium on photo-biochemistry in Yeungnam University, Republic of Korea on July 6<sup>th</sup>, 2017
- ***Functionality of Nanocomposites for environmental sustainability*** - International conference on Functional Materials in Thiagarajar College, Madurai, Tamilnadu, India during Sep 7-8, 2017.

#### Invited Talks as Plenary Speaker:

***New Insights on Photocatalysis*** – 3<sup>rd</sup> European Summer School on Advanced Oxidation Process, Universitat Politècnica De Valencia, Alcoy, Spain on June 5<sup>th</sup> 2019.

#### Organizing conference:

**Co-organizer:** Young Students Scientist Program (YSSP – 2012), Thiagarajar College, Madurai, Tamilnadu, India – from 09/05/2012 to 28/05/2012

#### Fellowships, Awards and Honors

**2014 – Excellent Paper Presentation Award** – Korean Society of Industrial and Engineering Chemistry conference

**2008 – Gold Medal** – Master of Science

**Date of Birth:** 30-07-1986

## References

1. **Prof. Suresh C. Pillai**,  
Head, Nanotechnology and Bio-Engineering Research Division,  
Department of Environmental Science,  
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Ash Lane, Sligo, Ireland  
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2. **Prof. Daphne Hermosilla**  
Associate Professor  
Vice-Dean of the School of Bioenergy,  
Department of Agricultural and Forest Engineering  
University of Valladolid  
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3. **Prof. Ir. Dr Srimala Sreekantan**  
Lecturer of School of Materials & Mineral Resources Engineering  
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### **Teaching Statement**

My academic carrier was started in 2008 as a lecturer in India. I have assigned to teach the course work and laboratory classes for the postgraduate and undergraduate students. I taught various courses such as Inorganic Chemistry, Industrial Chemistry, Analytical Chemistry, Environmental Chemistry, Water treatment, Nano-chemistry, Organic Chemistry, Physical Chemistry, Electrochemistry, *etc.* I taught a course entitled “Renewable Energy” for the doctoral students when I was working in the Republic of Korea. I have prepared the teaching portfolio for various subjects; this assists to develop my teaching abilities through systematic and rational planning. I have also served as a committee member to introduce new courses such as Diploma in Industrial safety and management, MSc Industrial Chemistry, and Certificate course in Chemical safety. I emphasize on theory, practical, communication and lifelong learning skills while teaching them. I use various pedagogical techniques such as lectures, laboratory exercises, student seminars, group presentation, *etc.* Exposure to research is an integral part of my teaching because the knowledge on course work is enhanced by understanding the techniques used to discover that information. Writing proficiency is a significant element of university education, and therefore all my courses are structured with writing assignments and a range of examination questions.

I have been evaluated by the students every year. I could manage to score above 90 % which has qualified me as a good teacher. I have developed practical pedagogical skills for creating inclusive learning environments for all students. For instant, cooperative learning, problem-based learning and tutorials are introduced for actively involving students in learning tasks; for encouraging students to work with each other. In doing so, I manage to provide opportunities for students to perform and receive suggestions for improvement and to accommodate the different talents and styles of learning for students.

For your more insight on my didactic skills please refer my lecture published in the YouTube <https://www.youtube.com/watch?v=2oauUVpQc7k> which was given for the Ph.D students at the 3rd European summer school on advanced oxidation process at Spain during June 2019.

### **Research Statement**

My doctoral research work describes the remediation of organic pollutants and heavy metals in water using semiconductor photocatalysis. The materials and technology developed in my research promote the national and international collaborations (Spain, Italy, India, Korea, Malaysia, and United Kingdom). Besides, these works have also promoted the level of thinking among researchers while elucidating scientific problems. In doing so, intelligent rationalisation and vindication in solving problems is cultivated among the researchers in my group. I am currently working in the EU-Interreg project at Institute of Technology Sligo (IT Sligo) in collaboration with University of Strathclyde (UK), South west College (UK), Kastus Ltd (Ireland) and Queens University Belfast (UK). This project is a €6 million cross-border collaboration project between the republic of Ireland, Scotland and Northern Ireland aimed at supporting technology development and knowledge transfer within the renewable energy and advanced manufacturing sectors.

My research works have been presented in many national and international level conferences (France, Canada, USA, Korea, etc). **My citations have been reached 1500 with an h-index of 24.**

#### ***Research Supervision and Evaluation:***

Through my research skills, I manage to supervise 10 postgraduate students in inorganic nano-chemistry at Master of Science level. Currently, I am co-supervising two Ph. D student's research work at IT Sligo. I have evaluated three Ph.D dissertations as an external examiner for Indian Universities. I have also evaluated three research proposals for funding from the government of Chile (Chilean National Science and Technology Commission), and Poland (National Science Centre). I am also acting as a committee member of Research and Innovation of Institute of Technology Sligo. I have given guest lectures to the researchers in various countries such as Korea, Spain, India, France, etc.

**Membership:** American Ceramic Society, European Microscopic Society, Irish Catalysis Society

**Research Plans:** Today, the global warming, energy crisis, infectious diseases and pollution are the serious threats to the humanity. My primary research goals are directed towards the development of nanoparticles for various applications like thermally stable energy storage devices, 2D membranes for water treatment, CO<sub>2</sub> capture and utilisation, hydrogen production from wastewater/seawater, electrocatalytic/PEC conversion of CO<sub>2</sub> into fuels and value-added products, antimicrobial food packing polymers, etc.

**Based on the research expertise, I am very much interested to extend my research work in the following areas:**

- Development of high temperature stable electrode and electrolytes for batteries and supercapacitors to address the fire explosion issues in electric vehicles and electronic devices.
- Design of antimicrobial food packing polymer films and indoor building materials to provide a hygienic health and protect us from life threatening infectious diseases. Also engineering of non-toxic antimicrobial coatings to the common touch screen surfaces, dental implants, and orthopedic implants.
- Development of 2D membrane materials for water treatment to remove persistent organic pollutants, infectious pathogens, and toxic heavy metals.
- Conversion of carbon dioxide ( $\text{CO}_2$ ) into fuels and value-added products.
- Renewable energy production in the form of hydrogen fuel from wastewater in a sustainable way. This would be beneficial to remove the impurities from wastewater and produce green energy using sunlight.
- Fabrication of self-cleaning coating from the agriculture waste. The content of silica is higher in sugarcane and rice husk ash.





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## Antimicrobial TiO<sub>2</sub> nanocomposite coatings for surfaces, dental and orthopaedic implants

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### ABSTRACT

Engineering of self-disinfecting surfaces to constrain the spread of SARS-CoV-2 is a challenging task for the scientific community because the human coronavirus spreads through respiratory droplets. Titania (TiO<sub>2</sub>) nanocomposite antimicrobial coatings is one of the ideal remedies to disinfect pathogens (virus, bacteria, fungi) from common surfaces under light illumination. The photocatalytic disinfection efficiency of recent TiO<sub>2</sub> nanocomposite antimicrobial coatings for surfaces, dental and orthopaedic implants are emphasized in this review. Mostly, inorganic metals (e.g. copper (Cu), silver (Ag), manganese (Mn), etc), non-metals (e.g. fluorine (F), calcium (Ca), phosphorus (P)) and two-dimensional materials (e.g. MXenes, MOF, graphdiyne) were incorporated with TiO<sub>2</sub> to regulate the charge transfer mechanism, surface porosity, crystallinity, and the microbial disinfection efficiency. The antimicrobial activity of TiO<sub>2</sub> coatings was evaluated against the most crucial pathogenic microbes such as *Escherichia coli*, methicillin-resistant *Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Bacillus subtilis*, *Legionella pneumophila*, *Staphylococcus aureus*, *Streptococcus mutans*, T2 bacteriophage, H1N1, HCoV-NL63, vesicular stomatitis virus, bovine coronavirus. Silane functionalizing agents and polymers were used to coat the titanium (Ti) metal implants to introduce superhydrophobic features to avoid microbial adhesion. TiO<sub>2</sub> nanocomposite coatings in dental and orthopaedic metal implants disclosed exceptional bio-corrosion resistance, durability, biocompatibility, bone-formation capability, and long-term antimicrobial efficiency. Moreover, the commercial trend, techno-economics, challenges, and prospects of antimicrobial nanocomposite coatings are also discussed briefly.

### 1. Introduction

The outbreak of various infectious diseases such as SARS-CoV, H1N1, and Ebola has resulted in a significant impact on the global economy and health systems [1,2]. SARS-CoV-2 is the most recent pandemic, caused by the human coronavirus [3–5]. The global mortality rate of SARS-CoV-2 is increasing everyday owing to its extremely contagious characteristics. At this stage, the world is fighting against an invisible enemy to control rampant infections and save lives. Studies are in progress on various aspects such as rapid detection, development of vaccines, medication, therapy, etc [6–8]. There is an urgent need to develop self-disinfecting surfaces to control the spread of this disease. Photocatalytic

surface coatings would be considered one of the best solutions to disinfect pathogens from the most commonly touched surfaces, such as commercial touch screens, mobile phones, ceramics, etc [9,10]. Non-toxic metal oxides are commonly used for photocatalytic coatings, which could respond to light and moisture to generate the reactive oxygen species (ROSs), to destroy the microbes. Compared to normal sanitation procedures, durable photocatalytic coatings could hinder the reactivation of microbes and destroy them completely. The mobility of ROSs in the air is normally higher and so it could effectively destroy airborne microbes [1]. Titanium dioxide or titania (TiO<sub>2</sub>) is one of the best photocatalysts for commercial antimicrobial coatings owing to its low-cost, reactivity, stability, reusability, durability, biocompatibility,

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# Solid Electrolytes for High-Temperature Stable Batteries and Supercapacitors

Vignesh Kumaravel,\* John Bartlett, and Suresh C. Pillai\*

Reports of recent fire accidents in the electronics and electric vehicles (EVs) industries show that thermal runaway (TR) reactions are a key consideration for the industry. Utilization of solid electrolytes (SEs) could be an important solution in to the TR issues connected to exothermic electrochemical reactions. Data on the thermal stability of modern SEs, ionic transport mechanisms, kinetics, thermal models, recent advances, challenges, and future prospects are presented in this review. Ceramic polymer nanocomposites are the most appropriate SEs for high-temperature stable batteries (in the range of 80–200 °C). Hydrogels and ionogels can be employed as stable, flexible, and mechanically durable SEs for antifreeze (up to –50 °C) and high-temperature (up to 200 °C) applications in supercapacitors. Besides the thermal safety features, SEs can also prolong the lifecycle of energy storage devices in next-generation EVs, space devices, aviation gadgets, defense tools, and mobile electronics.

## 1. Introduction

Thermal runaway (TR)-related explosions are the most common causes of fire accidents in batteries in the recent years.<sup>[1–3]</sup> TR normally occurs through uncontrolled or continuous exothermic reactions, and the increase of device temperature above 80 °C.<sup>[4]</sup> One well-publicized event of TR in electronic devices was the fire explosion issues of the Samsung Galaxy Note 7 in 2016. This resulted in severe economic losses for the Samsung company.<sup>[5,6]</sup> Batteries and supercapacitors are the most prominent electrochemical devices with distinct charge storage prop-


erties for various applications.<sup>[7–11]</sup> They are mostly fabricated using an anode, cathode, separator, and electrolyte. The schematic and mechanism of a battery (Figure 1a) and supercapacitor (Figure 1b) are displayed in Figure 1. Lithium (Li)-ion batteries are generally used in mobile phones, laptops, electric vehicles (EVs), etc.<sup>[12–14]</sup> Supercapacitors are employed in portable electronic devices, military tools, space devices, next-generation EVs, etc.<sup>[15–18]</sup> In any kind of electrochemical device, electrolyte is one of the most significant components to facilitate the ionic transport between the positive and negative electrodes.<sup>[19–22]</sup>

Liquid electrolytes (LEs) are preferred in traditional electrochemical devices to ease the ionic transport and wetting of the electrode surface.<sup>[23–25]</sup> Most LEs are made up of flammable organic solvents, such as ethylene carbonate (EC),<sup>[26]</sup> ethyl methyl carbonate (EMC),<sup>[27]</sup> and diethyl carbonate (DEC).<sup>[28]</sup> The failure of an electrochemical device under certain conditions could release flammable gases and this might trigger a fire hazard with the device at extreme temperatures.<sup>[29]</sup> Thermal decomposition of a battery or supercapacitor relies on its components, especially the electrolyte.<sup>[30,31]</sup> The characteristics of an electrolyte are more critical for high-temperature applications, compared to the electrodes or separators. The utilization of solid electrolytes (SEs) is an excellent choice to control the TR of an electrochemical device. SEs such as polymer electrolytes (PEs),<sup>[32,33]</sup> ceramic electrolyte (CE),<sup>[34,35]</sup> and ceramic-polymer electrolyte (CPE)<sup>[36,37]</sup> have been widely investigated in recent years. At high temperatures, the ionic conductivity and voltage safety window of SEs are superior when compared to LEs.<sup>[38]</sup> The important characteristics of the LE, PE, CE, and CPE are shown in Figure 2.<sup>[39]</sup> The flexibility, thermal stability, mechanical durability, electrochemical performance, ionic conductivity, interfacial contact, and Li dendrite suppression capability of CPE are superior, compared to LE, PE, and CE.

Generally, the CPE is composed of a polymer (e.g., polyvinylidene fluoride (PVDF)),<sup>[40]</sup> polyvinyl chloride,<sup>[41]</sup> poly(ethylene oxide) (PEO),<sup>[42]</sup> poly(methyl methacrylate), etc.,<sup>[43]</sup> Li salt (e.g., lithium bis(trifluoromethanesulfonyl)imide (LiTFSI)),<sup>[44]</sup> lithium bis(fluorosulfonyl)imide (LiFSI),<sup>[45]</sup> lithium perchlorate (LiClO<sub>4</sub>),<sup>[46]</sup> etc.), and a ceramic filler (e.g., aluminum oxide (Al<sub>2</sub>O<sub>3</sub>),<sup>[47,48]</sup> silicon dioxide (SiO<sub>2</sub>),<sup>[49]</sup> metal-organic frameworks (MOFs),<sup>[50]</sup> Li<sub>6.75</sub>La<sub>3</sub>Zr<sub>1.75</sub>Nb<sub>0.25</sub>O<sub>12</sub> (LLZNO),<sup>[51]</sup> Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub> (LLZTO),<sup>[52]</sup> etc.). The ceramic filler could be used in various dimensions such as 1D, 2D, and 3D (Figure 3).<sup>[39]</sup> The ionic conductivities of 2D and 3D materials are higher than that of 0D and 1D ceramic fillers.<sup>[39]</sup>

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# Plasmon-Induced Hot Electron Amplification and Effective Charge Separation by Au Nanoparticles Sandwiched between Copper Titanium Phosphate Nanosheets and Improved Carbon Dioxide Conversion to Methane

Jeong Yeon Do, Namgyu Son,<sup>#</sup> Rama Krishna Chava, Kotesch Kumar Mandari, Sadanand Pandey, Vignesh Kumaravel, T. S. Senthil, Sang Woo Joo, and Misook Kang\*

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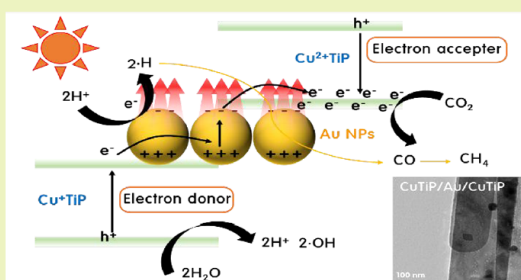
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**ABSTRACT:** Designing the catalysts to achieve the best performance is no exception in carbon dioxide (CO<sub>2</sub>) solar fuel conversion. Herein, we designed a CuTiP/Au/CuTiP catalyst, wherein gold (Au) nanoparticles were stably sandwiched between two copper titanium phosphate nanosheets (CuTiP). The catalyst was focused on the strong localized surface plasmonic resonance (LSPR) on the Au nanoparticles which led to the amplification of hot electrons between CuTiP nanosheets and the effective charge separation. The electrostatic force microscopy for CuTiP/Au provided the images of electrons that moved into the interface between the Au nanoparticle and CuTiP sheet as the voltage increases from 0 to 5.0 V. There was no product selectivity for the CO<sub>2</sub> conversion reaction on the CuTiP nanosheet, but the selectivity into methane (CH<sub>4</sub>) was significantly increased by anchoring Au nanoparticles. This was attributed to the effective charge separation on three phased surfaces formed between CuTiP, Au, and CuTiP, which led to excellent photocatalytic performance on CuTiP/Au/CuTiP. The density functional theory was used to support the proposed mechanism. The intensity-modulated photovoltage spectroscopy demonstrated that the recombination time between electrons and holes is remarkably slow on CuTiP/Au/CuTiP. Consequently, the designed catalyst in this study exhibited a CO<sub>2</sub> conversion performance at least 10 folds higher than those of previous catalysts in the gas-phase reactions, and deactivation of the catalyst was not found even after five recycling tests.

**KEYWORDS:** Au nanoparticle, Plasmon-induced hot electron amplification, Copper titanium phosphate nanosheets, Effective charge separation, Carbon dioxide conversion to methane



## INTRODUCTION

The sandwich composite consists of three or more layers of nanomaterials, and at least two layers of nanomaterials in contact are different. Thus, synergy between the two nanomaterials can be expected. Zaniewski and colleagues reported on electronic and optical properties of metal nanoparticle-filled graphene sandwiches.<sup>1</sup> They found that the presence of gold nanoparticles in the graphene sandwich sheet shifted the work function compared to unfilled bilayer graphene. Moreover, they confirmed that the sandwich compound filled with gold had the lowest resistance, and plasmon resonance was enhanced by coupling between metal nanoparticles present between two graphenes. In addition, Zhang et al. reported that graphene sandwich compounds encapsulated with Co<sub>3</sub>O<sub>4</sub> nanoparticles exhibit improved capacitor performance compared to pure Co<sub>3</sub>O<sub>4</sub> nanoparticles. Moreover, they obtained similar conclusions for sandwich compounds containing nickel nanoparticles prepared by the

same synthesis method.<sup>2</sup> In particular, Lv and colleagues found that the interfacial polarization (charge separation) and the stability of metal nanoparticles were significantly increased in the Ni/C nanoflakes material where Ni metal was sandwiched between carbon nanoflakes, and the microwave absorption characteristics were improved.<sup>3</sup> Recently, Liu et al. reported that it is possible to improve the activity and stability of heterogeneous catalysts by adjusting the atomic interface configurations of noble metals and transition metal oxides. It has been demonstrated that the interfacial sites formed

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# Photoelectrochemical Conversion of Carbon Dioxide (CO<sub>2</sub>) into Fuels and Value-Added Products

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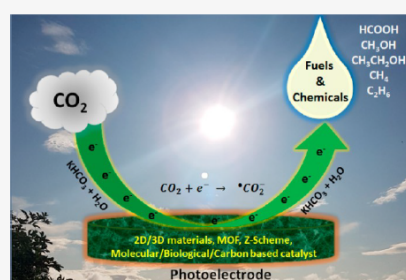
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**ABSTRACT:** The conversion of carbon dioxide (CO<sub>2</sub>) into fuels and value-added products is one of the most significant inventions to address the global warming and energy needs. Photoelectrochemical (PEC) CO<sub>2</sub> conversion can be considered as an artificial photosynthesis technique that produces formate, formaldehyde, formic acid, methane, methanol, ethanol, etc. Recent advances in electrode materials, mechanisms, kinetics, thermodynamics, and reactor designs of PEC CO<sub>2</sub> conversion have been comprehensively reviewed in this article. The adsorption and activation of CO<sub>2</sub>/intermediates at the electrode surface are the key steps for improving the kinetics of CO<sub>2</sub> conversion. PEC efficiency could be upgraded through the utilization of 2D/3D materials, plasmonic metals, carbon-based catalysts, porous nanostructures, metal–organic frameworks, molecular catalysts, and biological molecules. The defect engineered (by cation/anion vacancy, crystal distortion, pits, and creation of oxygen vacancies) 2D/3D materials, Z-scheme heterojunctions, bioelectrodes, and tandem photovoltaic–PEC reactors are suitable options to enhance the efficiency at low external bias.



Global warming, which results mainly from increased levels of atmospheric carbon dioxide (CO<sub>2</sub>), is one of the critical problems to emerge in recent years.<sup>1–4</sup> A large amount of CO<sub>2</sub> is released into the atmosphere every day in various ways, especially from the burning of fossil fuels. Dependence on fossil fuels not only intensifies the overuse of natural resources but also interrupts the carbon cycle.<sup>5–7</sup> Plants convert CO<sub>2</sub> into carbohydrates to maintain the carbon cycle by a process called photosynthesis, but this is significantly affected by the excess use of fossil fuels, deforestation, industrialization, and urbanization.<sup>8–10</sup> According to some projections, anthropogenic CO<sub>2</sub> levels could reach ~590 ppm by the year 2100, leading to an increase in the global temperature of 1.9 °C.<sup>11</sup> Most significantly, the temperature increase in the polar regions would be 3 times greater than that in other parts; this could severely impact the survival of all living beings on earth. The Paris agreement, which emerged from studies produced by the Intergovernmental Panel on Climate Change (IPCC), is intended to abate the net atmospheric CO<sub>2</sub> levels by 2050.<sup>12–14</sup> To address this, most countries have been taking numerous actions to develop renewable and sustainable energy production technologies.<sup>15</sup> CO<sub>2</sub> capture and utilization is a prime focus of research for the scientific community in recent years.<sup>16–21</sup> Various research

efforts have been established for capturing and sequestration of excess CO<sub>2</sub>.<sup>22–25</sup> The possibility of CO<sub>2</sub> leakage, high energy input, and complicated designs are major practical constraints of these methods.<sup>7</sup> Consequently, the recycling or conversion of CO<sub>2</sub> into fuels and other value-added products is an attractive option to address the global warming and energy crisis without impeding development and urbanization.<sup>26–37</sup>

Conversion of CO<sub>2</sub> is scientifically a challenging task, but it has significant benefits. Photoelectrochemical (PEC),<sup>38–42</sup> photocatalysis,<sup>43–48</sup> electrocatalysis,<sup>49–55</sup> thermocatalysis,<sup>56–61</sup> radiolysis,<sup>62–64</sup> and biochemical<sup>65–71</sup> techniques have previously been utilized for CO<sub>2</sub> conversion. Among them, PEC is identified as the ideal method to convert CO<sub>2</sub> into selective gaseous (e.g., methane, ethane, etc.) and liquid products (e.g., formate, methanol, ethanol, etc.) under solar light irradiation, especially for liquid products at ambient temperature and pressure.<sup>72–80</sup> This technology is also called artificial photosynthesis because it mimics nature's energy cycle.<sup>81–86</sup> PEC

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# Indium-Doped TiO<sub>2</sub> Photocatalysts with High-Temperature Anatase Stability

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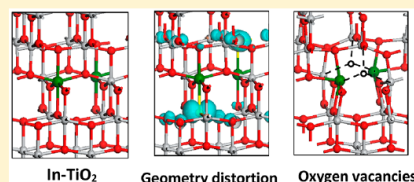
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**ABSTRACT:** The thermal stability of anatase titanium dioxide (TiO<sub>2</sub>) is a prerequisite to fabricate photocatalyst-coated indoor building materials for use in antimicrobial and self-cleaning applications under normal room light illumination. Metal doping of TiO<sub>2</sub> is an appropriate way to control the anatase to rutile phase transition (ART) at high processing temperatures. In this work, ART of indium (In)-doped TiO<sub>2</sub> (In–TiO<sub>2</sub>) was investigated in detail in the range of 500–900 °C. In–TiO<sub>2</sub> (In mol % = 0–16) was synthesized via a modified sol–gel approach. These nanoparticles were further characterized by means of powder X-ray diffraction (XRD), Raman, photoluminescence (PL), transient photocurrent response, and X-ray photoelectron spectroscopy (XPS) techniques. XRD results showed that the anatase phase was maintained up to 64% by 16 mol % of In doping at 800 °C of calcination temperature. XPS results revealed that the binding energies of Ti<sup>4+</sup> (Ti 2p<sub>1/2</sub> and Ti 2p<sub>3/2</sub>) were red-shifted by In doping. The influence of In doping on the electronic structure and oxygen vacancy formation of anatase TiO<sub>2</sub> was studied using density functional theory corrected for on-site Coulomb interactions (DFT+U). First-principles results showed that the charge-compensating oxygen vacancies form spontaneously at sites adjacent to the In dopant. DFT+U calculations revealed the formation of In - 5s states in the band gap of the anatase host. The formation of In<sub>2</sub>O<sub>3</sub> at the anatase surface was also examined using a slab model of the anatase (101) surface modified with a nanocluster of composition In<sub>4</sub>O<sub>6</sub>. The formation of a reducing oxygen vacancy also has a moderate energy cost and results in charge localization at In ions of the supported nanocluster. PL and photocurrent measurements suggested that the charge carrier recombination process in TiO<sub>2</sub> was reduced in the presence of In dopant. The photocatalytic activity of 2% In–TiO<sub>2</sub> calcined at 700 °C is more comparable with that of pure anatase.



## 1. INTRODUCTION

Titanium dioxide (TiO<sub>2</sub>) is one of the most popular nanomaterials in recent decades for its energy (solar cell,<sup>1</sup> water splitting,<sup>2</sup> CO<sub>2</sub> conversion/reduction<sup>3</sup>) and environmental (antimicrobial,<sup>4</sup> self-cleaning,<sup>5</sup> removal of toxic air/water pollutants<sup>6,7</sup>) applications under UV/visible light illumination.<sup>8</sup> Pure TiO<sub>2</sub> is commonly photoactivated by UV light owing to its wide band gap (3.2 eV for anatase and 3.0 eV for rutile phase TiO<sub>2</sub>).<sup>7,9</sup> Surface decoration<sup>10,11</sup> or inclusion of appropriate materials<sup>12–14</sup> in TiO<sub>2</sub> can favor its visible-light absorption for practical applications. Among the three crystalline phases of TiO<sub>2</sub> (such as anatase, rutile and brookite), the anatase phase shows maximum photocatalytic activity.<sup>15</sup> The lifetime of photogenerated charge carriers in the anatase phase is longer than that of rutile and brookite

phases.<sup>16</sup> However, many of the commercial TiO<sub>2</sub> products available in the market have a mixture of ~80% anatase and ~20% rutile phases (e.g., Degussa P25).<sup>17,18</sup> It is perceived that a mixed-phase composition of TiO<sub>2</sub> with a high percentage of anatase (more than ~60%) would reduce the charge carrier recombination process and enhance the photocatalytic efficiency.<sup>19</sup> Therefore, TiO<sub>2</sub> anatase could be used as an excellent additive in the manufacturing of building materials (especially ceramic tiles, sanitary ware, and glass) for indoor air purification, antimicrobial coatings, and self-cleaning surfaces under normal room light illumination.<sup>20–22</sup> However, most of these indoor building materials are processed and manufac-

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