

21st International Conference on

Advanced Energy Materials and Research

July 11-12, 2019 | Zurich, Switzerland

Scientific Tracks & Abstracts Day 1

Day-1

SESSIONS

Advanced Energy Materials | Solar Energy Materials | Advanced Graphene & 2D Materials | Advanced Nanomaterials | Hydrogen Energy and Fuel Cell Technology | Energy Harvesting Materials

Chair: Marie-Christine Record, Aix-Marseille University, France

Co-Chair: Mineo Hiramatsu, Meijo University, Japan

SESSION INTRODUCTION

Title: Investigation of the Culn_{1-x}Al_xSe₂ structure-properties relationships by coupling density functional and Bader's theories

Marie-Christine Record, Aix-Marseille University, France

Title: Electrochemically fabricated substrate dependent smart electrocatalysts Ni-Fe double and Ni-Co-Fe triple hydroxides for efficient water splitting to oxygen and hydrogen

Shahed U M Khan, Duquesne University, USA

Title: Synthesis of vertical graphene network as platform for electrochemical applications

Mineo Hiramatsu, Meijo University, Japan

Title: Magnetic instability in heavily n-doped Fe-based full Heusler compounds: Origin and

impact on thermoelectric properties

Fabio Ricci, University of Liège, Belgium

Title: Ceramic based thermoelectric materials processed by laser

N M Ferreira, Universidade de Aveiro, Portugal

Title: A framework for critically assessing the ideality of carrier-selective contacts for solar

cells

Gabriel J Man, Uppsala University, Sweden

Title: Photonic time crystal in exciton-polariton condensates

Szu-Cheng Cheng, Chinese Culture University, Taiwan

Title: Studies of (Pb, La)(Zr, Sn, Ti)O, antiferroelectric single crystal with high electrocaloric

effect

Qiang Li, Tsinghua University, China

Title: Solar PV/T integrated reversible solid oxide fuel cell system for power generation and

storage

S Ghosh, Indian Institute of Engineering Science and Technology, India

Title: Semiconductor nanostructure engineering for solar hydrogen production

Sabiha Akter Monny, The University of Queensland, Australia

Title: Magnesium ferrite/polyvinyl alcohol (PVA) nanocomposites: Fabrication and

characterization

Gulfam Nasar, Balochistan University of Information Technology, Engineering and

Management Sciences, Pakistan



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Investigation of the $CuIn_{1-x}Al_xSe_2$ structure-properties relationships by coupling density functional and Bader's theories

Marie-Christine Record¹, Pingping Jiang² and Pascal Boulet²
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For three decades density functional theory (DFT) has imposed itself as an accurate quantum method to investigate materials properties. In parallel, developments of density based descriptors such as Bader's quantum theory of atoms in molecules (QTAIM) brought new insights into the chemical bonding of materials. The ternary Cu-based chalcopyrite compound, CuInSe₂ (CIS), is an interesting material as solar cell absorber layer due to its low cost, high absorption coefficient, excellent optical and electrical properties. Many approaches have been adopted to improve its energy conversion efficiency. However, its narrow band gap and the scarcity and expensiveness of indium constrain its large-scale development. Replacing indium by the abundant and inexpensive aluminum to form the quaternary CuIn_{1-x}Al_xSe₂ (CIAS), has been considered as a promising alternative with few changes in physical and chemical properties. In this work, we investigated by DFT calculations the structural, electronic and optical properties of CuIn_{1-x}Al_xSe₂, for various "x" from 0 to 1, and determined the optimal substituting percentage. Moreover, in current PV cells, strains originating from the lattice mismatch between the PV materials and the substrates inevitably influence the optical performances, we calculated the band gap and optical properties for the optimal alloy subjected to biaxial strains. In the aim to unravel the deep relationship between bond interactions and optical properties, a detailed investigation of topological properties based on the electron density has been conducted as strain is applied.

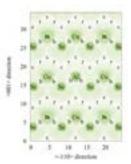


Figure: Electron density map with bond (b) critical points (CP) ring (r) CP and cage (c) CP.

- 1. H J Meadows, S Misra, B J Simonds, M Kurihara, T Schuler, V Reis-Adonis, A Bhatia, M A Scarpulla and P J Dale (2017) Journal of Materials Chemistry C 5:1336–1345.
- 2. O Meglali, A Bouraiou, N Attaf and M S Aida (2017) Optik International Journal for Light and Electron Optics 140:709–717.
- 3. K C Huang, C L Liu, P K Hung and M P Houng (2013) Applied Surface Science 273:723–729.

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- 4. W Deng, Z Yan, Y Fang and Y Wang (2014) Journal of Materials Science: Materials in Electronics 25: 2829–2834.
- 5. J López-García and C Guillén (2009) Thin Solid Films 517:2240–2243.
- 6. K W Cheng, K Hinaro and M P Antony (2016) Solar Energy Materials and Solar Cells 151:120–130.

Biography

Marie-Christine Record is Full Professor of Materials Chemistry at the University of Aix-Marseille, France since 2004. Her field of interest is solid state chemistry both from the experimental and computational stand points. Her experimental skills spread from the determination of phase diagrams and the synthesis of materials, by using methods as varied as mechanical alloying, self-propagating high temperature synthesis (SHS), reactive diffusion in thin films and electro chemical atomic layer epitaxy (EC-ALD), to materials structures (X-ray diffraction) and properties (electronic) characterization. For the purpose of better understanding the materials structure-properties relationships, she has developed for more than a decade computational strategies based on ab initio methods. She has been working on different kinds of materials such as intermetallics, chalcogenides for application purposes, especially for thermoelectric ones. She is author and co-author of more than 90 papers published in international scientific journals.

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Electrochemically fabricated substrate dependent smart electrocatalysts Ni-Fe double and Ni-Co-Fe triple hydroxides for efficient water splitting to oxygen and hydrogen

Shahed U M Khan and **Meron S Metaferia** Duquesne University, USA

Tater electrolysis is a significant method that can utilize renewable energy to produce hydrogen; a fuel that can transform earth towards a clean energy future. Activity of electrocatalysts for water oxidation is fundamental for energy conversion technologies including integrated solar power generating devices and water electrolyzers. In this study we have electrochemically fabricated the naturally abundant and stable electrocatalysts Ni-Fedouble hydroxides, Ni-Fe-Co-triple hydroxides, for efficient splitting of water to oxygen and clean fuel hydrogen. Oxygen-evolution activities of these electrocatalysts were examined in an alkaline solution of KOH. We focused in determining electro-catalytic activity of these double and triple hydroxides electrodeposited on different substrates such as Ni-foam, electrodeposited Ni-Co-oxide on Ni-foam and pressed porous Ni-Co oxide under varying electrodeposition bath composition, electrodeposition time and electrodeposition current and potentials. We found that Ni-Fe-Co triple hydroxide electrodeposited for total of 10 min on pressed porous Ni-Co-oxide sheet acted as a superior electrocatalyst for oxygen evolution reaction during water splitting reaction. This electrocatalyst generated a current density of ~ 100.0 mÅ cm⁻² at an oxygen overpotential of 0.270 volt (= 1.5-volt vs RHE) in 1.0 M KOH at electrolyte temperature of 25°C. However, this triple hydroxide deposited for 7 min generated 81.0 mA cm⁻² at the same overpotential, electrolyte concentration and temperature. The synergetic effect of multiple hydroxides and the substrates was mostly responsible for such enhanced electro-catalytic activity. The effect of higher electrolyte temperature was also found to have important role in enhancing the current density because of exponential dependence of reaction rate on temperature. The surface morphology and the composition of these electrocatalysts were determined using the scanning electron microscope (SEM) and energy dispersive spectroscopic (EDS) data.

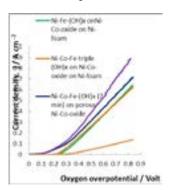


Figure: The oxygen evolution current density versus oxygen overpotential on Ni-Fe-double hydroxides and Ni-Co-Fe-triple hydroxides electrodeposited on various substrates such as Ni-foam, Ni-Co-oxide on Ni-foam and on pressed porous Ni-Co-oxide in 1 M KOH at electrolyte temperature of 25°C measured using the scan rates of 5 mV/sec

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 Khan S U M, Al-Shahry M and Ingler Jr W B (2002) Efficient Photochemical Water-splitting by Chemically Modified n-TiO₂. Science 297:2243-2245.

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- 2. Shabana Y A, El-Sayed M A, El-Maradny A A, Al-Farawati R K, Al-Zobidi M I and Khan S U M (2016) Photocatalytic removal of polychlorinated biphenyls (PCBs) using carbon-modified titanium oxide nanoparticles. Applied Surface Science 365:108–113.
- 3. Kavil Y N, Shaban Y A, Orif M I, Al-Farawati R, Zobidi M Khan and S U M (2018) Production of methanol as a fuel energy from CO, present in polluted seawater a photocatalytic outlook. Open Chem., 16:1089-1098.
- 4. Frites M, Ingler W B and Khan S U M (2014) A single chip standalone water splitting photoelectrochemical cell. I. Technol. Innov. in Renewable Ener., 3:6-11.

Biography

Shahed U M Khan has his expertise in the synthesis of materials for the electrochemical and photoelectrochemical splitting of water. He published more than 140 papers in various journals including some top ones such "Journal of Physical Chemistry", "Journal of American Chemical Society", "Journal of Electrochemical Society", "Chemical Physics, Applied Physics and Science". He co-authored books entitled "Quantum Electrochemistry", "Surface Electrochemistry" and coedited volume 7 of "Comprehensive Treatise of Electrochemistry." The focus of his research is to synthesize highly stable energy materials based on naturally abundant sources for efficient splitting of water to oxygen and hydrogen, a clean fuel to have carbon footprint free society in the planet Earth.

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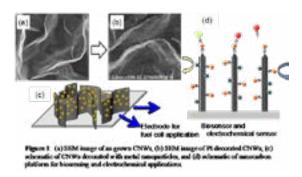
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Synthesis of vertical graphene network as platform for electrochemical applications

Mineo Hiramatsu Meijo University, Japan

raphene based materials such as carbon nanotube and graphene sheet itself have a wide range of possible Japplications. Among these grapheme based materials, carbon nanowalls (CNWs) are self- supported network of few-layer graphenes standing almost vertically on the substrate to form 3-dimensional structure. The mazelike architecture of CNWs with large-surface area graphene planes would be useful as electrodes for energy storage devices, electrochemical and biosensors and scaffold for cell culturing. CNWs and related materials can be synthesized by several plasma enhanced chemical vapor deposition (PECVD) techniques on heated substrates employing CH₄ and H₅ mixtures. Control of CNW structures including spacing between adjacent nanowalls and crystallinity is significant for the practical applications. Moreover, surface functionalization including surface termination and decoration with catalytic metal nanoparticles should be established. We report the current status of fabrication and structure control of CNWs using several PECVD techniques. Moreover, CNW surface was decorated with Pt nanoparticles by the reduction of chloroplatinic acid or by the metal-organic chemical deposition employing supercritical fluid. We also report the performances of hydrogen peroxide (H₂O₂) sensor and fuel cell, where CNW electrode was used. For the H₂O₃ sensing application, CNWs were grown on carbon fiber paper (CFP) using PECVD with CH₄/Ar mixture to increase the surface area. Then, CNW surface was decorated with Pt nanoparticles by the reduction of H,PtCl_c in solution. Cyclic voltammetry results showed that the Pt-decorated CNWs/CFP electrode exhibited excellent electrocatalytic activity to the reduction of H,O,. Similar structure was also used as a catalytic layer of the polymer electrolyte fuel cell. From the electrochemical investigation, Pt-decorated CNWs showed excellent electrochemical durability compared with the carbon black. Electrochemical experiments demonstrate that platform based on vertical nanographene offers great promise for providing a new class of nanostructured electrodes for electrochemical sensing and energy conversion applications.



Recent Publications

1. Imai S, Kondo H, Hyungjun C, Ishikawa K, Tsutsumi T, Sekine M, Hiramatsu M and Hori M (2019) Pt nanoparticle-supported carbon nanowalls electrode with improved durability for fuel cell applications using C₂F₂/H₂ plasma-enhanced chemical vapor deposition. Applied Physics Express 12:015001.

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- 2. Tomatsu M, Hiramatsu M, Foord J S, Kondo H, Ishikawa K, Sekine, M Takeda K and Hori M (2016) Hydrogen peroxide sensor based on carbon nanowalls grown by plasma-enhanced chemical vapor deposition. Japanese Journal of Applied Physics 56:06HF03.
- 3. Watanabe H, Kondo H, Okamoto Y, Hiramatsu M, Sekine M, Baba Y and Hori M (2014) Carbon nano wall scaffold to control culturing of cervical cancer cells. Applied Physics Letters 105:244105.
- 4. Hiramatsu M and Hori M (2010) Carbon nanowalls: synthesis and emerging applications. Springer Verlag Wien.
- 5. Hiramatsu M, Shiji K, Amano H and Hori M (2004) Fabrication of vertically aligned carbon nanowalls using capacitively coupled plasma-enhanced CVD assisted by hydrogen radical injection. Applied Physics Letters 84:4708-4710

Biography

Mineo Hiramatsu is a Full Professor of Department of Electrical and Electronic Engineering and the Director of Research Institute, Meijo University, Japan. He served as the Director of The Japan Society of Applied Physics. His main fields of research are plasma diagnostics and plasma processing for the synthesis of thin films and nanostructured materials. He served as Chairman and Member of organizing and scientific committees of international conferences on plasma chemistry and plasma processing. He was awarded the Japan Society of Applied Physics Fellow in 2017.

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Magnetic instability in heavily n-doped Fe-based full Heusler compounds: Origin and impact on thermoelectric properties

Fabio Ricci, Sébastien Lemal, Matthieu J Verstraete and Philippe Ghosez University of Liège, Belgium

re, YZ full Heusler compounds, on which first principles on density functional theory (DFT) simulations predict Γ very large thermoelectric power factor (PF), are promising candidates for thermoelectric applications. The building blocks of their interesting thermoelectric properties are the carriers belonging to the Fe-eg orbitals that can be opportunely engineered to maximize PF. These anti-bonding states are represented by a flat band (mainly composed of Fe dx^2-y^2 character) along the ΓX direction of the Brillouin Zone, related to the highly directional Fe-Fe bond, becoming dispersive along the other directions. This band satisfies the "flat-and-dispersive" requirements proposed by Mahan and Sofo and leads to one-dimensional transport strongly enhancing the PF. However, due to its strongly localized nature, explicit n-doping may induce a Stoner instability driving the system to a half-metallic phase. The present study, performed through DFT using both hybrid functional and GGA+U methods on Fe, YZ, A_x (Y = Ti, V, Nb, Ta, Z=Al, Si, Sn, Ga and A=Si, P, Sb, Ge) n-doped systems, shows that the appearance of such a magnetic phase is strictly linked to the Fe-eg and Y-site eg orbital hybridization and that it possesses a pure electronic origin, independent on the dopant species. Although the Stoner instability can provide half-metallicity with coupled thermomagnetic responses, the PF is typically reduced in the half-metallic phase due to a reduction of the number of carriers available at the Fermi level. In certain cases, however, the values of the PF are still large (for Fe, TaGa, _Ge_ or Fe, TiSi, P, PF is between 9 and 15 10⁻³ W K⁻² m⁻¹ at 600 K, for example) which stays promising for thermoelectric applications. Going further, we elucidate the possibility to exploit the broader nature of 4d and 5d orbitals at the bottom of the conduction band to overcome the magnetic phase appearance in the doping range of interest.

Biography

Fabio Ricci did his PhD on both simulations and experimental measurements on magnetic properties of materials (diluted magnetic semiconductors and soft magnetic materials) by means of the magneto-optical Kerr effect. Subsequently, he worked on theoretical simulations on Fe-based superconductors, principally iron-chalcogenides. He developed and implemented in the ABINIT code the formalism for the non-collinear magnetism in the density functional perturbation theory and, at the same time, started to work on the theoretical engineering of thermoelectric properties of the Fe-based full-Heusler compounds.

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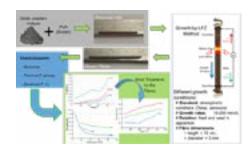
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Ceramic based thermoelectric materials processed by laser

N M Ferreira¹, M A Madre², A Sotelo², A V Kovalevsky¹ and F M Costa¹ Universidade de Aveiro, Portugal ²ICMA, CSIC-Universidad de Zaragoza, Spain

Today a particular interest is given to the oxide-based thermoelectric materials, due to enhanced thermal and redox stability, attractive properties at high temperature, together with the absence of toxicity, and natural abundance of the constituent compounds. The objective of this work is to assess the possibilities for processing oxide thermoelectrics through laser floating zone (LFZ) method, including identification of the appropriate treatment conditions and main structural and microstructural factors affecting the thermoelectric performance. Known that Nb and La substituted calcium manganite-based materials possesses promising thermoelectric properties, they were selected as a model system. Detailed structural (XRD) and microstructural (SEM/EDS) studies were performed for the samples grown at various pulling rates. The results on electrical conductivity, Seebeck coefficient and thermal conductivity indicate that high thermoelectric performance can be triggered by laser processing. Effects of pulling rate, dopants nature and thermal treatment to the fibres on that properties are discussed, suggesting that careful optimization of the laser treatment conditions is necessary, when seeking high thermoelectric performance in oxides by LFZ processing.



- 1. N M Ferreira, F M Costa, A V Kovalevsky, M A Madre, M A Torres, J C Diez and A Sotelo (2018) New environmentally friendly Ba-Fe-O thermoelectric material by flexible laser floating zone processing. Scripta Materialia 145:54–57.
- 2. N M Ferreira, M C Ferro, A R Sarabando, A Ribeiro, A Davarpanah, V Amaral, M A. Madre, A V Kovalevsky, M A Torres, F M Costa and A Sotelo (2018) Improvement of thermoelectric properties of Ca0.9Gd0.1MnO₃ by powder engineering through K₂CO₃ additions. Journal of Materials Science 54:3252–3261.
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- 4. A Sotelo, F M Costa, N M Ferreira, A Kovalevsky, M C Ferro, V S Amaral, J S Amaral, S Rasekh, M A Torres, M A Madre and J C Diez (2016) Tailoring Ca₃Co₄O₉ microstructure and performances using a transient liquid phase sintering additive. J. Eur. Ceram. Soc. 36 1025.

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5. M A Madre, F M Costa, N M Ferreira, S I R Costa, Sh Rasekh, M A Torres, J C Diez, V S Amaral, J S Amaral and A Sotelo (2016) High thermoelectric performance in Bi_{2-x}Pb_xBa₂Co₂O_x promoted by directional growth and annealing. Journal of the European Ceramic Society 36:67-74

Biography

N M Ferreira is a PhD in Physics Engineering; currently is a Researcher at i3N, Physics Department at University of Aveiro, Portugal. He had participated in several R&D projects on Material Science. He have experience as researcher in study and development of ceramics-based materials, prepared through conventional methods by melting, solid stated, with particular focus on laser processing (crystal growth – LFZ and surface sintering/modification). Present sample characterization skills include various techniques such as, electrical conductivity and magnetic properties of various oxide materials. Current focus materials are thermoelectrics, ferroelectrics and glass matrices doped with transition metals and rare earth for energy storage and conversion applications. Main expertise is related to structural, magnetic and electrical properties of materials prepared by laser processing.

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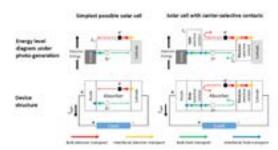
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A framework for critically assessing the ideality of carrier-selective contacts for solar cells

Gabriel J Man

Uppsala University, Sweden

The simplest solar cell consists of a light absorber, sandwiched between two metals with dissimilar work functions. Carrier-selective contacts (CSC's), which are ubiquitous in modern solar cells, are added to improve the electrical performance. The proper design and implementation of a CSC is crucial, as the performance, lifetime, and/or cost reduction of a solar cell can be hampered by a single interface or layer. A framework, consisting of eight core requirements, was developed from first-principles to evaluate the effectiveness of a given CSC. The framework includes some requirements which are well-recognized, such as the need for appropriate band offsets, and some requirements which are not well-recognized at the moment, such as the need for effective valence/conduction band density of states matching between the absorber and CSC. The application of the framework to multiple silicon-based CSC's revealed the difficulties of effectively designing and implementing a CSC. Three metal oxide/silicon heterojunctions - titanium dioxide/silicon (TiO₂/Si), zinc oxide/silicon (ZnO/Si), and tin dioxide/silicon (SnO₂/Si) - initially expected to yield similar electron-selective contacts (ESC's) were instead discovered to be widely different in terms of their suitability as an ESC.



- 1. G J S Man (2017) Metal oxide/semiconductor heterojunctions as carrier-selective contacts for photovoltaic applications. Princeton University.
- 2. G Man, J Schwartz, J C Sturm and A Kahn (2016) Electronically passivated hole-blocking titanium dioxide/silicon heterojunction for hybrid silicon photovoltaics. Adv. Mater. Interfaces 3(15):1600026.
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- 4. G Sahasrabudhe et al., (2015) Low-Temperature Synthesis of a ${\rm TiO_2}$ /Si Heterojunction. J. Am. Chem. Soc., 137(47):14842-14845.
- 5. S Avasthi, W E McClain, G Man, A Kahn, J Schwartz and J C Sturm (2013) Hole-blocking titanium-oxide/silicon heterojunction and its application to photovoltaics. Appl. Phys. Lett., 102(20):203901.

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Biography

Gabriel Man has worked as a Postdoctoral researcher in the Division of Molecular and Condensed Matter Physics at Uppsala University since April 2018. In his current work, he applies and develops X-ray spectroscopic techniques to gain fundamental understanding of the relationships between the crystal and electronic structures of advanced energy materials. His work spans both fundamental and applied science, and is guided by his background in engineering and technology entrepreneurship. Prior to his postdoctoral appointment, Gabriel spent nearly a year working in industry as a device engineer/physicist at a thin film solar cell startup company. Gabriel received his PhD in 2017 in Electrical Engineering and Materials Science from Princeton University (New Jersey, USA) under the supervision of Prof Antoine Kahn. His PhD research was partially supported by a prestigious PhD fellowship from the Natural Sciences and Engineering Research Council of Canada (NSERC), and by a fellowship from Princeton University.

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Photonic time crystal in exciton-polariton condensates

Szu-Cheng Cheng

Chinese Culture University, Taiwan

A many body state, which has symmetry different from the true quantum ground state of the Hamiltonian is referred to a state with spontaneous symmetry breaking. The usual crystals in the material science own a kind of discrete spatial translation symmetry and show the spontaneous symmetry breaking of continuous spatial translation symmetry. Recently, a new kind of crystal, called a time crystal, was shown a crystalline structure formed in the time domain due to the spontaneous breaking of continuous time translation symmetry. Time crystals could only exist in non-equilibrium many body systems. A exciton-polariton condensate existing in a microcavity is intrinsically out of equilibrium so that continuous pumping is needed to balance the fast polariton decay and maintain a steady-state state. Here, we propose a photonic time crystal occurring in exciton-polariton condensates and a method to realize it experimentally. We find that a resonantly-pumped exciton-polariton condensate subjected to an external periodic potential could show a spontaneous time-symmetry breaking and lead to the formation of a time crystal. We also study the effects of light frequency detuning on the periodicity of the time crystal. The proposed time crystals of a resonantly-pumped exciton-polariton condensate provide a new horizon for exploring properties of matter and its possible application in quantum computations.

Recent Publications

- 1. Ting-Wei Chen and Szu-Cheng Cheng*, "Surface gap solitons in exciton polariton condensates.", 2018, Physical Review E, 98, 032212.
- 2. Szu-Cheng Cheng and Ting-Wei Chen*, "Dark gap solitons in excitonpolariton condensates in a periodic potential", 2018, Physical Review E, 97, 032212.
- 3. Ting-Wei Chen and Szu-Cheng Cheng*, Polariton solitons and nonlinear localized states in a one-dimensional semiconductor microcavity.", 2018, Physical Review E, 97, 012218.
- 4. Szu-Cheng Cheng* and Shih-Da Jheng, "Physical Realization of von Neumann Lattices in Rotating Bose Gases with Dipole Interactions.", 2016, Scientific Reports, 6, 31801.
- 5. Ting-Wei Chen, Shih-Da Jheng, Wen-Feng Hsieh, Szu-Cheng Cheng*, "Nonequilibrium and nonlinear defect states in microcavity-polariton condensates," 2016, Physical Review E, 93, 052214.
- 6. Ting-Wei Chen, Wen-Feng Hsieh and Szu-Cheng Cheng*, "Stable gray soliton pinned by a defect in a microcavity-polariton condensate", 2015, Optics Express, 23, 24974.

Biography

Szu-Cheng Cheng is a Professor and Chairman for the Department of Optoelectric Physics of Chinese Culture University in Taiwan. He has his expertise in theoretical studies of photonic crystals and Bose-Einstein condensates. He is a Member of the American Physical Society and the American Optical Society. His multiple-fluxes vortex-lattice model shows new pathways for creating new matter state. He has built this model after years of experience in research and teaching in education institutions. He is a specialist in condensed matter physics. Currently, his research interest is on the physical phenomena of exciton-polariton condensates in microcavity of quantum wells.

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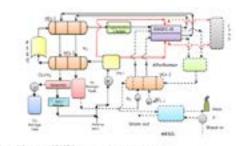
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Solar PV/T integrated reversible solid oxide fuel cell system for power generation and storage

S Ghosh, A Ghosh and A K Mishra

Indian Institute of Engineering Science and Technology, India

In this paper, a novel power generation cum storage system employing reversible solid oxide fuel cell (RSOFC) has been proposed. The RSOFC is integrated with solar PV/T system that also includes parabolic trough solar collectors (PTSC). The RSOFC unit operates in steam electrolyser mode (during day time) and in fuel cell mode (during night time). The electrochemical model is developed for a proton conducting reversible solid oxide fuel cell (RSOFC-H) and its performance analysis is done both in fuel cell mode and electrolysis mode of operation. A comparative performance analysis has also been done between conventional oxide ion conducting reversible SOFC (RSOFC-O) and proton conducting RSOFC-H for suitably chosen range of current density to cover both the cells' common operating range (500 A/m² to 5000A/m²). Computational simulation model for the integrated plant has been developed and the simulated performance analyzed both using energy and exergy approaches. The results suggest that the solar-integrated system can yield an overall solar-to-gas conversion efficiency of about 18% in electrolysis mode while in fuel cell mode the conversion efficiency (gas-to-power) would be about 40%.



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- 1. Saetova N S, Krainova D A, Kuzmin, A V, Raskovalov A A, Zharkinova S T, Porotnikova N M and Ghosh S (2019) Alumina–silica glass–ceramic sealants for tubular solid oxide fuel cells. Journal of Materials Science 54(6):4532-4545.
- 2. Huang N, Zhao P, Ghosh S and Fedyukhin A (2019) Co-hydrothermal carbonization of polyvinyl chloride and moist biomass to remove chlorine and inorganics for clean fuel production. Applied Energy 240:882-892.
- 3. Roy D, Samanta S and Ghosh S (2019) Techno-economic and environmental analyses of a biomass based system employing solid oxide fuel cell, externally fired gas turbine and organic Rankine cycle. Journal of Cleaner Production.
- 4. Roy D, Samanta S and Ghosh S (2019) Energetic, exergetic and economic (3E) investigation of biomass gasification-based power generation system employing molten carbonate fuel cell (MCFC), indirectly heated air turbine and an organic Rankine cycle. Journal of the Brazilian Society of Mechanical Sciences and Engineering 41:112.

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Biography

S Ghosh is an Associate Professor in the Department of Mechanical Engineering, Indian Institute of Engineering Science and Technology, Shibpur. He received his Bachelor of Engineering (Mechanical) from University of North Bengal, India, in 1991, Master of Engineering (Heat Power) from Calcutta University, in 1993 and PhD from Jadavpur University in 2005. Besides having a two-decade long teaching and research experience, his career includes industrial work experience at ABB ABL, Durgapur, India (later taken over by Alstom Power). His areas of research include Clean Coal Technology, Renewable Energy Technologies like Fuel Cells, Biomass Gasification and Greenhouse Technology. He is closely associated with a few renewable energy research groups in Europe, USA and Canada and he has served as Guest Scientist at Paul Scherrer Institute (PSI), Switzerland (during 2006 and 2007), where his focus of work was development and technology demonstration of biomass gasification integrated fuel cell (SOFC) system.

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Semiconductor nanostructure engineering for solar hydrogen production

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Photoelecctrochemcial water splitting provides an attractive method to convert the abundant solar energy into sustainable and clean hydrogen energy. The greatest challenge is how to develop efficient and stable photoelectrodes, including photoanodes and photocathodes. Comparing to the widely studied photoanodes, the photocathodes have been paid less attention due to the scarcity of suitable semiconductor candidates. Some available photocathodes derived from p-type semiconductors such as single crystal Si, chalcogenide (e.g., CuInGaSe) are either not stable or too expensive to realize large scale application. Herein, a promising p-type semiconductor, CuBi₂O₄, has been used to fabricate efficient photocathode. Moreover, combining the CuBi₂O₄ photocathode with well-developed BiVO₄ photoanode, it is able to demonstrate unbiased sunlight-driven solar water splitting. CuBi₂O₄ electrodes were prepared with electrodeposited BiOI and copper acetylacetonate as precusor after heating in air at 450°C for 4 hours. The CuBi₂O₄ photocathode possesses a porous nano branch strucutre and showed a photocurrent of -0.95 mA/cm² at 0.21 VRHE along with an onset potential at 1.1 VRHE in Sodium Phosphate (~pH 7) electrolyte. With the presence of electron scavengers, the photocurrent was further enhanced to -2.4 mA/cm² at 0.48 VRHE. The incident photon-to-current efficiency showed a threshold at ca. 620 nm, suggesting a broad light harvesting range of the CuBi₂O₄ photocathode. Furthermore, the large onset potential of CuBi₂O₄ photocathode makes it feasible to realize unbiased photoelectrode water splitting when combined with suitable photoanode, such as BiVO₄.

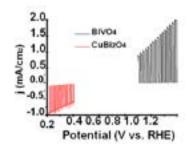


Figure: The photoresponse of CuBi2O4 and BiVO4 under chopped light

Biography

Sabiha Akter Monny is a PhD student at the University of Queensland. She specialises in renewable energy, energy conversion and nanomaterials. Her research focuses on developing photocatalysts using semiconductor nanomaterials for photoelectrochemical energy conversion.

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