



THEME:

Renewable and Sustainable Energy from the African Hot Sun: Can Materials Chemistry Help to Deliver?

INTERNATIONAL CONFERENCE ON MATERIALS CHEMISTRY, 2016

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BOOK OF ABSTRACTS

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Introduction

Ready availability of energy plays a pivotal role in economic and social development of all countries around the world. Access to cheap energy has brought great economic prosperity to many countries especially in the developed world. Many of the current sources of energy used globally have negative impacts on the environment. Hence there is ongoing debate about making energy systems more environmentally benign and sustainable. The discussion has largely centred on the nature of different energy sources and their likely impact on the environment. In the search for alternative energy, solar energy occupies an important place since it is abundant. However, it is not easily and economically exploited at the moment.

In Africa, electrical energy is often inaccessible, unaffordable, or unreliable for many people. The availability of electricity supply in Africa lags far behind that of other continents. This limits development: students find it difficult to read after dark, clinics cannot refrigerate vaccines and businesses have shorter operating hours. Power rationing has become a common phenomenon in many African countries due to insufficient power generation. This affects the running of pieces of equipment which require 24 h power supply, leading to frequent breakdown of such equipment and interruption of some research programmes.

Solar resource is by far the single most abundant energy resource Africa has and if harnessed could meet all the electricity needs of Africa. Solar energy, falling freely from Africa's skies to reach everywhere on the continent without transmission lines can be utilized to provide off-grid electricity to remote communities far from national grids, as well as utility scale electricity for industries. The challenge, however, is that the present cost of converting the solar energy to electricity and other forms of energy for easy use is prohibitive. New materials to efficiently absorb sunlight, new techniques to harness the full spectrum of wavelengths in solar radiation, and new approaches based on nanostructured architectures can revolutionize the technology used to produce solar electricity. The technological development and successful commercialization of single-crystal solar cells demonstrate the promise and practicality of photovoltaics, while novel approaches exploiting thin films, organic semiconductors, dye sensitization, and quantum dots offer fascinating new opportunities for cheaper, more efficient, longer-lasting systems. These can offer a future for the utilization of solar energy which abounds in large quantities into energy for sustainable development.

The main objective of this conference is to emphasize the importance of and showcase new developments in materials chemistry and its possible role for harnessing solar energy and providing energy for sustainable development. It is also aimed at promoting novel research and collaborations on materials chemistry by bringing together experts and interested parties from all over the world and from diverse bodies – from the academia to the industry and to governments.

Subthemes

Topics to be discussed at the conference will include:

- 1 Harnessing Solar Energy for Sustainable Development
- 2 Materials for Harnessing Renewable Energy from the Sun
- 3 Inorganic Nanomaterials for Solar Cell Applications
- 4 Organic / Conducting Materials for Solar Cell Applications
- 5 Hybrid Solar Cell Materials for Energy Applications
- 6 Fabrication of Solar Cell Materials for Energy Applications
- 7 Renewable/Alternative Energy from Biomass

Scientific Committee

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Dr. Marian Asantewah Nkansah, Department of Chemistry, KNUST, Kumasi, Ghana

Dr. Mrs. Mercy Badu, Department of Chemistry, KNUST, Kumasi, Ghana

Programme

Day One (03 October 2016)

10:00 – 11:30 Opening Session: (To include a keynote address and Photographs)

10:00	Opening Prayer	
10:05	Introduction of Chairman and Dignitarie	es
10:10	Chairman's Response	Prof (Mrs) Ibok Oduro
		Provost, College of Science, KNUST
10:20	Welcome Address	Prof. Kwesi Obiri Danso
		Vice-Chancellor, KNUST
10:30	Introduction to the Conference	Chairman, LOC of Conference
10:40	The Role of the RSC in Promoting	Dr Helen Driver, Senior Manger
	Science for Sustainable Development	Royal Society of Chemistry, UK
10:50	Keynote Address based on main theme	Minister for Environment, Science, Technology and Innovation, Ghana
11:10 11:20	Chairman's Closing Remarks Vote of Thanks	Prof (Mrs) Ibok Oduro
11:25	Closing Prayer	
11:30	Break for Group Photographs and Snach	XS
11:30 - 12:00	Snack Break	
12:00 - 13:00	Plenary Lecture on "Harnessing Solar Kwame Ampofo , Chairman, Energy Co	r Energy for Sustainable Development" By Dr pmmission, Ghana
13:00 - 14:30	Lunch	
14:30 - 15:30	Plenary Lecture on "Materials for Harn Paul O'Brien , CBE, FRS, University of	essing Renewable Energy from the Sun" By Prof f Manchester, UK
15:30 - 16:15	Keynote Oral Presentation on "Polyn	her Solar Cells – from fundamental aspects to

15:30–16:15 Keynote Oral Presentation on "Polymer Solar Cells – from fundamental aspects to technological breakthrough" By **Dr. Hanne Lauritzen**, Special Advisor, Technical University of Denmark (DTU), Institute for Energy Conversion and Storage, Denmark

16:15 – 16:45 Break for Beverages

16:45 – 17:30 Oral Presentations

- 1. Investigation of the Efficient Conversion of Photon Energy to Electricity by Newly Synthesised Well-Ordered Low Band Gap Semiconducting Organic Molecules - Boniface Y. Antwi
- 2. Computational Study on Transition Metal Catalysts for CO2 Conversion to Hydrocarbon Fuels-

Caroline R. Kwawu

18:30 Cocktail

Day Two (04 October 2016)

- 8:30 9:30 Plenary Lecture on Renewable Energy from Biomass by **Dr. Essel Ben Hagan**, Adjunct Associate Professor, KNUST, Kumasi
- 9:30 10:15 Keynote Lecture on Synthesis of Cellulosic Polymer Composites and Possible Applications – **Prof. Tshwafo E. Motaung**, Head, Chemistry Department, University of Zululand, South Africa

10:15 – 11:00 Oral Presentations

- 1. Synthesis and Characterization of CaO from Guinea Fowl Egg Shells (GFESS) M-M Pedavoah
- 2. A Simple Chemical Route Synthesis and Characterization of CuO Nanoparticles; Material for Photo Electronic and Photovoltaic Applications A. A. Yankson
- 3. Lead Xanthate Complexes: Efficient Single Source Precursor Route to PbS Nanowires Selina Ama Saah

11:00 - 11:30 Break

- 11:30 13:00 Oral Presentations
- 1. Castor Oil and Olive Oil: Towards a Greener Synthesis of Nanostructured In_2S_3 Siphamandla C. Masikane
- 2. Synthesis of CdS Nanoclusters and PbS Nanobelts from Ethylxanthate Single Source Precursors (SSP) using the Heat-Up Technique and Castor Oil as Solvent- Michael B. Mensah
- 3. Investigating Some Structural Properties of Mn Doped ZnO Nanoparticles Synthesized by the Solution and Solid State Techniques E. A. Armah

13:00 - 14:30 Lunch

14:30 – 15:30 Plenary Lecture on Organic/Conducting Polymers for Solar Cells by **Prof. Peter Skabara**, University of Strathclyde, Glasgow, Scotland, UK

15:30 – 17:00 Oral presentations

- 1. Effect of Precursors on the Morphology and Electronic Properties of CdS Nanoparticles Kevin I. Y. Ketchemen
- 2. Anti-MoS₂ Material: 2D Nanosheets of Acanthite by Liquid Phase Exfoliation Malik Dilshad Khan
- 3. Pd Decorated ZnS/RgO Nanocomposite for Enhanced Visible-Light-Driven Photocatalytic Activity towards Indigo Carmine Eric S. Agorku

- 4. Green Synthesis of Palladium Nanoparticles for Catalytic Application Ayorinde. O Nejo
- 17:00 18:00 Break and Poster Session
- 18:00 Break for Conference Dinner

Day Three (05 October 2016)

8:30 – 9:30 Plenary Lecture on Inorganic Materials for Solar Cells by Prof Neerish Revaprasadu, SACHI Chair of Nanotechnology, University of Zululand, South Africa

9:30 – 11:00 **Oral Presentations**

- 1. Iron Sulfide Thin Films and Nanoparticles for Potential Applications in Gas Sensing Sixberth Mlowe
- 2. Heterocyclic Bismuth(III) Dithiocarbamato Complexes as Single-Source Precursors for the Synthesis of Anisotropic Bi₂S₃ Nanoparticles Walter N Kun
- 3. Heterocyclic Dithiocarbamates: Precursors for Shape Controlled Growth of CdS and PbS Nanoparticles Linda Dyorisse Nyamen
- 4. Developing Functional Nanomaterials Containing Phthalocyanines for Various Applications Ruphino Zugle
- 11:00 11:30 Break
- 11:30 12:30 Plenary Lecture on Fabrication of Solar Cell Materials for Energy Applications, By Dr John Thomas Prabhakar, University of Bangor, Bangor, Wales, UK
- 12:30 13:30 Flash Poster Presentations
- 13:30 14:30 Lunch
- 14:30 15:30 Closing Ceremony

ORAL PRESENTATIONS

O-1 Novel Approaches to Complex Quantum Dot Structures

Paul O'Brien

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Abstract

We have been interested over a number of years in developing novel chemical methods to both new and better known materials as both thin films and particles with critical dimensions of the order of nanometers. Some of these routes have been, or are being exploited, in a range of commercial applications. The ability to convert molecules to materials led, in the 1990s, to new methods for the preparation of particles with critical dimensions of the order of nanometers. When such materials are constructed from a semiconductor the electronic properties of the particle become dependent upon its size; because of guantum confinement. Such particles are hence termed 'guantum dots'. Their unique properties especially efficient luminescence has led to their potential for use in display technologies. A current interest involves, studying the internal structures of more complex structures; those involving more than one component. A variety of spectroscopic and microscopic methods have been used to probe such structures. A second related interest concerns quantum dots made from complex or more difficult materials such as those with several potential phases such as iron or copper sulfides or of complex composition such as the kesteritic phases (CZTS) or their more complex derivatives. The direct preparation of polymer composites of such compounds is also a current area of interest. Many of these materials have potential commercial application notably in photovoltaic solar cells.

O-2 Polymer Solar Cells – From Fundamental Aspects to Technological Breakthrough

Hanne Lauritzen

Special Advisor, Technical University of Denmark (DTU), Institute for Energy Conversion and Storage

Abstract

Of all known renewable energy technologies the polymer solar cell is the only one that inherently enables fast manufacture of an energy-producing unit with a sub-µm thin outline and using abundant materials only. The majority of the research in its field has, however, not been devoted to unlocking this potential, but to improving its power conversion efficiency following the scientific tradition of conventional PV technologies. The effort has paid off, and power conversion efficiencies exceeding the 10% claimed possible about 10 years ago has been demonstrated - a scientific hallmark in its own right. But as the archetypal solar cell studied is prepared in tiny formats under inert conditions by using techniques that are not scalable, a complementary approach is needed for substantiating the polymer solar cell's technological reality. DTU's mission is to develop polymer solar cell into a winning PV technology, and we are doing so by turning tings upside down and refocus at the polymer solar cell in the form we would ideally like to apply it and also how we ideally prepare it. From this position we specify the technical requirements set to the solar cell and its manufacturing process, and subsequently we trace these backwards to the design of the solar cell's architecture and its materials and forwards to the deployment and end-of-life phase. The talk will present highlights from DTU's work that spans the entire value chain from cradle to grave.

O-3 Investigation of the Efficient Conversion of Photon Energy to Electricity by Newly Synthesised Well-Ordered Low Band Gap Semiconducting Organic Molecules.

Boniface Y. Antwi¹, Rupert G. D. Taylor², Richard B. Owoare¹, Robert K. Adaboh¹ and Peter J. Skabara².

¹Department of Chemistry, University of Ghana, Legon-Accra, Ghana, byantwi@st.ug.edu.gh ²Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow, United Kingdom.

Abstract

Demand for carbon free energy has grown over recent years as the world fights against climate change. Current reports show that conventional energy production has environmental and economic challenges associated with it. Consequently, much attention has been directed towards harvesting solar energy for electricity generation. This alternative source of energy is expected to be a sustainable and greener source compared to current methods. Even though progress has been made in this direction, there is much room for improvement. For instance, the prevailing high cost of silicon based solar cells has necessitated varied research into affordable alternative photoactive materials with high power conversion efficiencies. A promising area amongst these is organic photoactive materials (both polymers and small molecules). They have unique properties such as, flexibility, large area applicability, ease of processing and low cost. Research shows that, efficiency of these materials correlates with mobility of photogenerated charge carriers. Ultrafast photo-induced charge transfer (< 100 fs) is best achieved in the bulk-heterojunction solar cell architecture with networked domains (10-20 nm in size) of donor and acceptor materials. The ability of an acceptor material to form networked domains is much desired and pursued in current global research. These domains form from the self-assembling of molecules into perfect crystals. It is therefore inferred that, crystalline molecules enhance charge carrier mobility prior to recombination in organic solar cells. Therefore, it is imperative that, newly synthesised donor molecules crystallise for efficient charge transfer. In all, our work seeks to explore the unique features of terthiophene (Figure 1) derivatives and their self-assembling properties, without sacrificing spectral absorption abilities in the synthesis of novel low band gap semiconducting molecules for application in organic solar cell technology.

Keywords: energy, solar, photovoltaic, semiconductor, and molecules.

O-4 Computational Study on Transition Metal Catalysts for CO₂ Conversion to Hydrocarbon Fuels

<u>Caroline R. Kwawu¹</u>, Richard Tia^{1*}, Evans Adei¹, Nelson Y. Dzade², C. Richard A. Catlow^{3,4} and Nora H. de Leeuw ^{2,3,4}

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³Department of Chemistry, University College London, 20 Gordon Street, WC1H 0AJ, London, UK. ⁴School of Chemistry, Cardiff University, Main Building, Park PI, Cardiff CF10 3AT, UK.

Abstract

The search for renewable energy sources and CO₂ pollutions necessitate CO₂ transformation to fuels but this has been challenging due to the stability of the CO₂ molecule. Despite the industrial challenges with CO₂ reduction, metal clusters composed of both iron (Fe) and nickel (Ni) have been found in nature as active electro-catalytic sites. Thus, surface modification of iron with nickel could enhance catalytic applications. One of the promising paths to CO₂ mitigation is via the production of CO, a feedstock, in the Fischer–Tropsch process for the synthesis of long chain hydrocarbons. This paper reports the result of the DFT study into the energetics of the conversion of CO2 into fuels on clean iron surfaces and the effect of nickel deposition on the surface catalytic properties, so as to provide mechanistic insights into the process. Nickel deposition reduces the work function on the (110) surface indicating that CO₂ activation and reduction should be more feasible on the nickel deposited (110) surface. CO₂ chemisorbs on all three low Miller indices of iron and its decomposition is thermodynamically most favoured on the flat, most closed packed (110) facet. However, the activation barrier for both activation and dissociation tends to be highest on that facet, directly related to its high surface work function. This suggests that kinetically, dissociation is least favoured on the most stable (110) facet which is the most expressed facet of iron as observed in the Wulff's morphology plot. The reverse water gas shift reaction on clean iron will proceed via the carboxyl intermediate and a modified surface which provides lower barrier leading to dihydroxyl carbonyl formation will improve yields on the iron surface. Our calculations indicate that CO₂ dissociation is most challenging on the (110) facet due to the high surface work function on that facet. Work function of the (110) facet could be reduce by nickel deposition, which is most enhanced at the least 0.25 ML coverage. This findings have implications for the development of improved Fe electro-catalysts (for example CO2 reduction).

KEY WORDS: DFT, Nickel deposition, Work function, Reverse water-gas shift mechanism

O-5 Synthesis of Cellulosic Polymer Composites and Possible Applications

<u>Tshwafo E. Motaung</u>^{*}, Linda Z. Linganiso, Rakesh Kumar and Rajesh D. Anandjiwala

Department of Chemistry, University of Zululand, Private Bag X1001, Kwa-Dlangezwa, 3886, South Africa.

Abstract

Agave Americana (agave) and Agave sisalana (sisal) fibers belong to the same family of natural fibers. Both the fibers were treated with alkali. Interestingly, alkali treated agave fibers displayed a clean and smooth surface whereas alkali treated sisal fibers showed a rough surface due to the rupture of alkali sensitive bonds. This indicated that the sisal fibers are more susceptible to alkali treatment as compared to agave fibers. The experimental studies of chemical composition, Fourier transform infrared spectroscopy (FT-IR) and X-Ray diffraction (XRD) were also carried out. Both alkali treated agave and sisal fibers were used to reinforce polyfurfuryl alcohol (PFA) matrix. The effect of these fibers on the mechanical and thermo-mechanical properties of PFA composites was examined. Mechanical, thermal and thermo-mechanical properties of the composites were studied. The results indicated the improvement in mechanical and thermal properties of the reinforce PFA.

O-6 Synthesis and Characterization of CaO from Guinea Fowl Egg Shells (GFESS)

M-M. Pedavoah^{1,2}, J.A.M. Awudza², M. Badu², N.O. Boadi²

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²Kwame Nkrumah University of Science and Technology (Kumasi), College of Science, Department of Chemistry, Ghana

Abstract

Annually, millions of tons of various egg shells go waste across the world. These can be channeled into useful materials with adequate research and development. Guinea fowl egg shells (GFESs) were collected from domestic kitchen waste and processed for synthesis. The GFESs were calcined at varying temperatures of 700, 800, 900, 1000 and 1100 °C respectively for two hours in a muffle furnace. The raw or uncalcined GFESs and the calcined GFESs were characterized by FTIR, TGA and XRD analyses. The uncalcined GFESs showed intensive peaks at wave numbers that corresponded to CaCO₃ phases which transformed into Ca(OH)₂ as the temperature of calcination increased and finally to CaO. The XRD defractograms presented main peaks at 2 theta values of 29.466 for the uncalcined GFESs and 37.377 for the sample calcined at 1100°C. Using the Scherer equation, the crystallite sizes ranged from 18.9 - 50.68 nm. All the samples showed a two-step decomposition pattern, with a weight loss of up to 47%, which was mainly due to the removal of moisture and organic components. The sample calcined at 1100 °C showed mainly CaO phases in the XRD analysis and was fairly stable with only 7% loss in weight after treatment at 800°C

Key words: calcined guinea fowl egg shells, CaCO₃, TGA, FTIR, XRD.

O-7 A Simple Chemical Route Synthesis and Characterization of CuO Nanoparticles; Material for Photo Electronic and Photovoltaic Applications

A. A. Yankson, A. Kuditcher, G. G. Hagos, and J. K. Amuzu

Department of Physics, University of Ghana, Legon

Abstract

A simple inexpensive chemical route has been identified and used to synthesize cupric oxide nanoparticles suitable for photo electronic and photovoltaic applications. X-ray diffraction analysis showed the synthesized nanoparticles to be a pure cupric oxide phase. The particle size and particle size distribution of the cupric oxide nanoparticles were obtained by transmission electron microscopy (TEM) whereas the crystallite size and crystallite size distribution were obtained by X-ray diffraction peak broadening analysis. The particle size was found to be between 20 nm and 60 nm, an indication that cupric oxide nanoparticles are dominant in the sample produced and analysed. The particle size distribution obtained from cumulative percentage frequency plots features a Gaussian distribution. Absorbance measurements and analysis show that the material has an absorbance peak around 314 nm and an average energy bandgap of 1.48 eV showing a strong potential for photo electronic and photovoltaic applications.

O-8 Lead Xanthate Complexes: Efficient Single Source Precursor Route to PbS Nanowires

Selina Ama Saah¹, Johannes A. M. Awudza¹ and Neerish Revaprasadu²

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Department of Chemistry, University of Zululand, Private Bag X1001, KwaDlangezwa, 3886, South Africa.

Abstract

Lead alkyl xanthate (alkyl = octyl, nonyl and dodecyl) complexes have been synthesized by reacting lead acetate trihydrate with the corresponding alkyl xanthate ligand. The complexes were characterized by micro-elemental analysis, infrared spectroscopy and thermogravimetric analysis. The complexes were then used as single source precursors for the syntheses of PbS nanowires through by decomposition in olive oil media, using hot injection techniques. The synthetic route adheres to basic principles of green chemistry, since olive oil is non-toxic and the thermolysis was performed at moderate reaction temperatures. The influence of the alkyl chain length of the single source precursor and temperature on the properties of the PbS nanowires has been studied. Powder X-ray diffraction (p-XRD) analyses of the as-synthesized nanowires corresponded to a cubic rock salt (halite) PbS structure. Transmission electron microscope (TEM) images of the as-synthesized nanomaterials showed a 1-dimensional growth of nanowires with length of ca. 80 nm and width of ca. 10 nm. Energy dispersive X-ray spectroscopy (EDX) showed approximately 1:1 Pb:S ratio in the as-synthesized nanowires. The estimated band gaps from the Tauc plots were 1.34, 1.41 and 1.47 eV for PbS nanowires obtained from octyl, nonyl and dodecyl chain lengths respectively indicating a significant blue shift relative to the bulk band gap of 0.41 eV.

Keywords: lead xanthate, single source precursors, hot injection, lead sulfide, nanowires

O-9 Castor Oil and Olive Oil: Towards a Greener Synthesis of Nanostructured In₂S₃

Siphamandla C. Masikane,^a David J. Lewis,^b Paul O'Brien,^b Neerish Revaprasadu^a

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(b) School of Materials, University of Manchester, Oxford Road, Manchester, M13 9PL, United Kingdom

Abstract

Alternatives to toxic semiconductor materials and their fabrication processes have become a priority in the material sciences and engineering research communities. An appropriate example is indium sulfide, a relatively nontoxic semiconductor material which has been identified as a worthy candidate to replace the toxic CdS as a photocatalyst [1], as well as being a buffer layer in cadmium gallium indium sulfide/selenide solar cells [2]. We report a greener synthesis of nanostructured In_2S_3 through a one-step solvothermal decomposition of a known single-source molecular precursor, *tris*-ethlyxanthato indium (III). Powder x-ray diffraction, ultraviolet-visible-near infrared spectroscopy and transmission electron microscopy are amongst techniques which were used to evaluate the influence of varying reaction temperature and type of green passivating agent on the properties of the as-prepared In_2S_3 nanostructures.

Keywords: CuO, inexpensive chemical route, particle size, crystallite size, absorbance peak, average band gap

O-10 Synthesis of CdS Nanoclusters and PbS Nanobelts from Ethylxanthate Single Source Precursors (SSP) using the Heat-Up Technique and Castor Oil as Solvent

Michael B. Mensah, Johoannes A. M. Awudza

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Abstract

Castor oil is a non-edible vegetable oil which has been extensively employed as raw material in the synthesis of biodegradable polymers. However, it has currently gain attention as a readily available, relatively inexpensive, and environmentally friendly solvent for semiconductor nanoparticles synthesis. Thus, we report the synthesis of CdS nanoclusters and PbS nanobelts via a simple heat-up of ethylxanthate single source precursors (SSP) in castor oil. The synthesized SSPs were directly thermolyzed in castor oil to obtain the nanoparticles. The nanoparticles were characterized with X-ray diffractometer (XRD), UV-Visible spectrophotometer (UV-Vis), photoluminescence (PL) spectrophotometer, scanning electron microscope – energy dispersive X-ray spectroscope (SEM/EDXS) and transition electron microscope (TEM). The CdS showed a bandgap of 2.63 – 2.73 eV and a strong PL emission in the near-UV. The CdS were nanoclusters of spherical particles with average size of 6.78±1.89 nm whilst PbS showed a nanobelt morphology with some nanosquare discs. The average width and length of the PbS nanobelts were 22.19+2.33 nm and 225.94+23.32 nm respectively. The average bandgap of the PbS was 0.85 eV. Elemental analysis showed that the CdS composed of 49.74 % Cd and 50.49 % S whilst the PbS consisted of 49.42 % Pb and 50.58 % S. Thus, using simple heat-up technique and castor oil as an environmentally benign solvent, useful morphologies of CdS and PbS were obtained.

Keywords: Heat-up, hot-injection, synthesis, single source precursor, ethylxanthate, nanocrystals, castor oil

O-11 Investigating Some Structural Properties of Mn Doped ZnO Nanoparticles Synthesized by the Solution and Solid State Techniques

E. A. Armah¹, F. K. Ampong¹, R. K. Nkum¹ and J. K. Amuzu²

¹Department of Physics, Kwame Nkrumah University of Science and Technology, Kumasi ²Department of Physics, University of Ghana, Legon

Abstract

The effect of doping on the crystal structure of Mn-doped ZnO nanoparticles synthesized by the solution and solid phase techniques have been studied by Powder X-Ray diffraction. The nanoparticles were synthesized at temperatures of 160 °C and 180 °C. Results showed that the nanoparticles synthesized by both techniques had the wurtzite structure with well-defined peaks. For the films synthesized at 180 °C, secondary peaks were observed in the diffractogram when the doping concentration exceeded 20 % for the solid phase method, and 10 % for the solution phase method. There were no traces of Mn detected in the diffraction patterns below these limits however there were irregular shifts in the peak positions. For the synthesis at 160 °C, secondary peaks appeared in the diffractogram with doping concentrations as low as 0.5 % for the solution phase and 2.5 % for the solid phase. The Mn-doped ZnO nanoparticles prepared by the solution method were generally found to have bigger crystallite size than those prepared by solid phase method at both temperatures.

O-12 To Bend or Not To Bend - Designing Optimal Conformations in Conjugated Macromolecules for Organic Photovoltaic Devices

Peter J. Skabara

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Abstract

The control of molecular architecture in organic semiconductors is a highly important aspect of organic electronics. This is particularly the case for planar conjugated structures to enhance charge transport and obtain low band gap materials. The goal of this lecture is to present a solid argument, based on a combination of experimental data and modelling, for the importance of heteroatomic non-classical bonds in conjugated organic molecules and macromolecules and to provide an insight to design rules for the manipulation of chemical structure towards targeted properties. Whilst potential noncovalent interactions can be easily identified in molecular structures determined by single crystal X-ray diffraction (XRD) studies, it is significantly more difficult to prove such interactions exist in polymers. A combination of XRD experiments on model structures, spectroscopy and computational studies can be a means to such an end, especially if the materials under study are members of a generic structure in which only the heteroatoms differ. The main question answered here is whether heteroatomic non-covalent interactions are coincidental or real, or if the sole driver for planar architectures in conjugated molecules is hydrogen bonding. A combined approach using experiment and theory clearly shows that heteroatom interactions are significantly influential.

Keywords: conjugated macromolecules, self-assembly, organic photovoltaics

O-13 Effect of Precursors on the Morphology and Electronic Properties of CdS Nanoparticles.

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Abstract

Cadmium sulfide (CdS) is one of the most studied semiconductor with a direct band gap energy of 2.42 eV which is widely used in various applications such as photocatalyst, optoelectronic devices, solar cell panel and LED display devices.¹ Under thermal conditions, the morphology, size and phase of nanostructured materials are influenced by reaction parameters such as passivating groups, monomer concentration, and temperature and precursor type. As a simple, easy controlled, low cost and effective heating method, thermal decomposition of single source precursors (SSP) in coordinating solvents have been widely used in the synthesis of nanomaterials.^{2,3} The synthesized complexes, cadmium dihexyl dithiocarbamate (1), cadmium diethyl dithiocarbamate (2), cadmium ethyl xanthate (3) and cadmium piperidine dithiocarbamate (4) were characterized by elemental analysis, FT-IR spectroscopy and thermo gravimetric analyses. The complexes were used as single source precursors for the synthesis of CdS nanoparticles in hexadecylamine (HDA) and oleylamine (OLA) at 250 °C. Spherical and oval shaped particles with sizes ranging from 12.80 ± 4.36 to 17.83 ± 4.26 nm were obtained in OLA while spherical, oval and rods shaped particles with sizes ranging from 11.52 ± 2.72 to 28.42 ± 4.79 nm were obtained in HDA. UV/visible spectra of the nanoparticles showed a blue shift compared to bulk CdS, with the OLA capped nanoparticles more blue shifted than the corresponding HDA capped nanoparticles. The p-XRD patterns revealed the hexagonal crystal structure of CdS. For the same reaction parameters, smaller particles were obtained from the xanthate complexe compared to the dithiocarbamate complexes.

O-14 Anti-MoS₂ Material: 2D Nanosheets of Acanthite by Liquid Phase Exfoliation

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Abstract

After the discovery of graphene and the amazing properties associated with it for advanced technological applications, layered 2 dimensional materials have attracted worldwide attention.^{1,2} The bulk layered crystals are composed of stacked layers which have strong covalent bonding within the layers but interconnected by each other by weak Vander Waals force of attraction. The layers can be separated easily by breaking the Vander Waals interaction between the layers. Transition metal dichalcogenides have sandwich like structure in which the transition metal atom is sandwiched between two chalcogenide atoms.³ Silver sulfide has an interesting structure which is inverse to transition metal dichalcogenides i.e. chalcogen is sandwiched between two silver atoms. It was observed that the Aq-Aq contacts between two adjacent layers is equal to Vander Waals distance and can be exfoliated. Such sheets with anti-MoS₂ structure may exhibit interesting unique properties. Herein, we report the synthesis and characterization of 2D silver sulfide nanosheets. Silver sulfide was synthesized by solventless decomposition of (O-ethyldithiocarbonato) silver (I) complex. The bulk silver sulfide generated was exfoliated using NMP to obtain nanosheets. The size and thickness of the sheets was determined by scanning electron microscopy and atomic force microscopy respectively. We believe that it would be a valuable addition to the 2D materials.

O-15 Nanomaterials Synthesis: Issues of Precursors, Green Chemistry and Simplicity

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Abstract

The talk will focus on recent work done in my laboratory on the synthesis of semiconductor nanomaterials. I will discuss the recent synthesis of new complexes which have been used to prepare iron, bismuth, antimony and tin chalcogenide nanomaterials. The lecture will also focus on the use of green materials as capping groups for nanoparticles. The use of anarcardic acid and castor oil will be discussed in detail. Finally I will show how you can use simple reactions to prepare nanomaterials.

O-16 Pd Decorated ZnS/RgO Nanocomposite for Enhanced Visible-Light-Driven Photocatalytic Activity towards Indigo Carmine

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Abstract

The removal of toxic organic pollutants from wastewater using reduced graphene oxide (rGO)-based photocatalysts has dominated recent scientific research. As a result numerous nanomaterials have been studied and used for wastewater remediation. ZnS has been widely studied due to their versatile application in photcatalysis. This study presents the synthesis of a series of Pd-decorated ZnS/rGO nanocomposites by coprecipitation method. The materials were characterized using Raman spectroscopy, Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM)-EDS and UV/Visible spectrophotometry. Indigo carmine (IC) dye (20 ppm) was chosen as a model for organic pollutants and was used to evaluate the photocatalytic performance of the Pd-ZnS/rGO nanocomposites under visible light with varying concentrations of Pd in the host material. Pd-ZnS/rGO showed significant visible light induced photocatalytic activity towards the degradation of IC. Highest photocatalytic activity was observed for the 1.0 % Pd-ZnS/rGO sample ($k = 2.19 \times 10^{-2} \text{ min}^{-1}$).

Keywords: photodegradation, palladium, reduced graphene oxide, ZnS, indigo carmine

O-17 Green Synthesis of Palladium Nanoparticles for Catalytic Application

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Abstract

Palladium nanoparticles (PdNPs) were synthesised using aqueous extract of ginger (Zingiber Officinale) and Tumeric (Curcuma longa), which acts as both reducing and stabilizing agent. After the reduction of Pd²⁺ to Pd⁰ the PdNP's were characterised using UV-Vis spectroscopy, Fourier transformations infrared spectroscopy. The prepared Palladium Nanoparticles were used as a catalyst.

Keyword: Palladium nanoparticles, Ginger, Turmeric, Catalyst

O-18 Iron Sulfide Thin Films and Nanoparticles for Potential Applications in Gas Sensing

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Abstract

Iron sulfide nanomaterials are interesting class of nanomaterials and play a role in materials science like solar cells, biological and other applications. The crystal structure and phase transformations of iron sulfide nanomaterials are complex [1,2]. Iron (III) complexes piperidine (1) and tetrahydroquinoline (2) dithiocarbamate have been synthesized, crystal structures elucidated and subsequently utilized as single source precursors for the preparation of iron sulfide thin films and nanoparticles by chemical deposition and thermolysis methods, respectively. The sizes and shapes of crystallites obtained by AACVD method depended on the nature of the precursor, temperature, solvent and the amount of *tert*-butyl thiol used. Iron sulfide nanoparticles Fe₃S₄ and Fe_{1-x}S were synthesized via solvothermal decomposition of heterocyclic iron(III) dithiocarbamate complexes in oleylamine. At a reaction temperature of 230 °C, the cubic Fe₃S₄ phase (greigite) was obtained whereas at 300 °C, monoclinic Fe₁₋ $_{\rm x}$ S (pyrrhotite) was obtained. In both cases, hexagonal sheet like structures with sizes ranging from 50 – 200 nm were obtained. Powder X-ray diffraction studies reveal that the temperature plays a significant role in determining the crystalline structure and chemical composition of the as-synthesized nanoparticles (NPs). The magnetic properties of the nanoparticles were also temperature and phase-dependent. Gas sensing applications further reveal activities which are phase-dependent. The greigite has a higher response to humidity but saturates faster than the pyrrhotite. The pyrrhotite phase however outwits the greigite on response to H₂, NO₂, NH₃ and CH₄. In these gases, the greigite displays early saturation as well as noisy and uncoordinated signals.

O-19 Heterocyclic Bismuth(III) Dithiocarbamato Complexes as Single-Source Precursors for the Synthesis of Anisotropic Bi₂S₃ Nanoparticles

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Abstract

The morphology, size and phase of nanostructured materials are influenced by reaction parameters such as passivating groups, monomer concentration, temperature and precursor type. Simple, easy controlled, low cost and effective heating method such as thermal decomposition of single source precursors (SSP) in coordinating solvents have been widely used in the synthesis of high quality nanomaterials. Bismuth sulfide (Bi₂S₃) is a direct band semiconductor (1.3 to 1.7 eV), widely used as a thermoelectric-cooling material, in photovoltaic converters and photodiode arrays. We report the synthesis and characterization of catena-(μ_2 -nitrato-O,O')bis(piperidinedithiocarbamato) bismuth(III)) (1) and tetrakis(µ-nitrato)tetrakis [bis(tetrahydroquinolinedithiocarbamato) bismuth(III)] (2) Bi (III) complexes. They were characterized by elemental analysis, FT-IR spectroscopy, thermo gravimetric and single X-ray crystal analyses. Both complexes were used as single source precursors for the synthesis of dodecylamine (DDA), hexadecylamine (HDA), oleylamine (OLA) and tri-n-octylphosphine oxide (TOPO) capped Bi₂S₃ nanoparticles at different temperatures. UV/vis spectra showed blue shift in absorption band edge characteristic of a quantum size confinement in the particles. The p-XRD patterns revealed the orthorhombic crystal structure of Bi₂S₃. Elongated crystals and short nanorods shaped Bi₂S₃ were obtained at different temperatures. The shape of the nanomaterials was affected by the thermolysis temperature ranging from 190 °C to 270 °C. A general trend of increase in the particle size with an increase of the reaction temperature as well as the length of the carbon chain of capping agent was observed.

Keywords: Single Source precursors, nanoparticles, Bismuth Sulfide

O-20 Heterocyclic Dithiocarbamates: Precursors for Shape Controlled Growth of CdS and PbS Nanoparticles.

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Abstract

Amongst the many methods reported for the synthesis of anisotropic CdS nanoparticles, the use of single source precursors containing both the metal and the sulfide source has proven to be an effective route to high quality nanoparticles. In spite of their toxic nature, several research groups are engaged in the preparation and characterization of lead (II) nanostructured semiconductors such as PbS, PbSe, PbTe, from single source molecular precursor due to their potential applications in optoelectronic devices. CdS is one of the metal chalcogenide materials which shows a variation in 1D morphology when the reaction conditions change (nature of capping agent, reaction temperature and reaction time). However the control of the dimensions of the CdS rods is still a challenge. The diameter of the nanoparticles is often too large to exhibit quantum confinement. We report the synthesis of organically- capped CdS and PbS nanoparticles using cadmium piperidine dithiocarbamate and cadmium tetrahydroquinoline heterocyclic dithiocarbamate complexes as single source precursors. These complexes are easy to prepare, air stable for long periods and pyrolyze to give high guality nanoparticles. The nanoparticles obtained showed quantum confinement with near band edge luminescence. The reaction conditions such as the amount, type of capping group and reaction temperature were varied to study their influence on the properties and final morphology of the nanoparticles. Elongated CdS particles in the form of rods, bipods and tripods, were obtained. For PbS, particles in the shape of cubes and rods were obtained. The CdS and PbS particles were characterized by X-ray diffraction and electron microscopy techniques.

O-21 Developing Functional Nanomaterials Containing Phthalocyanines for Various Applications

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Abstract

The properties and applications of phthalocyanines have largely been assessed in various solvent media. However, most applications of phthalocyanines are preferable in their solid state as in read-write compact disc or when incorporated into solid support systems. Such support systems offer some comparably better advantages such as ease of recovery of the phthalocyanine during photocatalysis. Support systems such as zeolite and polycrystalline titanium dioxide have been ambelite, reported. Functionalization of electrospun nanofibers through the integration of functional molecules such as phthalocyanines into polymer nanofiber core, are often desirable in fields such as biosensor technology, tissue engineering, drug delivery, heterogeneous catalysis and nano-electronics. The current project is focussed on the incorporation of functional phthalocyanines molecules into solid electrospun polymer nanofibers through covalent linkages as well as vander waals interactions. This is followed by assessment of the photochemical and photophysical properties of the phthalocyanine in the resulting fabric materials. The resulting functionalised nano-materials are then applied for gas sensing, removal of environmental organic pollutants and also as antibacterial and antifungal agents.

O-22 Nanocrystal "Inks" for Solar Energy Generation Applications

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Abstract

Nanocrystal arrays could yield a low-cost, low-tech route to solar cells. A topical challenge in the area is to device interconnects to produce a hybrid layer capable of harvesting light. This talk will summarize the advantages of nanocrystalline assemblies and attempt to provide a snapshot of the state of the art in ligand engineering to obtain optimal performance for nanocrystalline arrays.

POSTER PRESENTATIONS

P-1 Morphological Evaluation of Hematite Nanostructures on FTO Substrate by Organic Templating

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Abstract

World reserves of fossil energy such as petroleum, gas and coal are depleting rapidly. Viable alternative energy sources include; hydroelectric, geothermal, solar, nuclear, biomass and wind. Among these, conversion of solar energy by photovoltaic technology has become quite apt. Semiconductor materials such as; titanium dioxide (TiO2), zinc oxide (ZnO), stannic oxide (SnO2), and iron oxide (α -Fe2O3) known as hematite are candidate photoanode materials in Dye Sensitized Solar Cells (DSSC). Hematite compared to the rest has smaller optical band gap of ca 2.2 eV making it favourable for photocatalytic, photoelectrochemical and photovoltaic applications. In this study hydrothermal synthesis were achieved on FTO glass starting from precursor iron compounds to give initially the iron oxyhydroxides (β -FeOOH) before annealing in air to afford the hematite nanostructures. The nanostructures were characterized using SEM-EDX, XRD and AFM. It was observed that morphology of the hematite nanostructures were influenced by the organic templates; PEG, CTAB, PVP, UREA, PMMA, Boric acid and Polyacrylamide respectively. The shapes obtained include nanowires, some in ball shaped or blocky clusters. The average height from AFM was in the range of 3-4 nm. The morphological control of the nanostructures observed in this study can be a viable approach to tune the photoelectrochemical properties of hematite semiconductor materials for DSSC applications.

Keywords: Nanowires, Hematite, Photovoltaic, Photoanode, Surfactant templating

P-2 Biodiesel Production from Castor, Coconut and Jatropha Oils Using Calcined Oyster Shells and Naoh as Catalysts

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Abstract

Biodiesel are composed of fatty acid methyl esters (FAMEs). FAMEs were produced through the transesterification of coconut, castor and jatropha oils using calcined oyster shells and NaOH as catalysts. Using 2% catalyst amount of the oil weight for both oyster shells (calcined at 1000°C for 2.5 hours by a Thermal Gravimetric Analyzer (TGA)) and NaOH, transesterification was carried out under reflux at 1:6 oil to methanol ratio, a temperature of 80°C and a reaction period of 6 hours to produce biodiesel. Thin Layer Chromatography (TLC) was then used to confirm the reaction completion. Castor oil produced the maximum biodiesel yield; 92% for calcined oyster shells and 84% for NaOH catalyst. Jatropha oil had the lowest biodiesel yield of 86% for oyster shell and 73% for NaOH catalyst. NaOH was less efficient to transesterify the oils as compared to the oyster shells. The FAMEs were analyzed by a Varian CP-3800 GC with Hydrogen as the carrier gas at 1.4 ml/min and identified with known standards. Heterogeneous oyster shell catalyst for biodiesel production.

P-3 Investigation on the Global Phase Diagrams with a Re-Entrant Transition Behaviour

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Abstract

In this paper we calculate the global phase diagrams with the closed-loop behavior for the phase transition of systems by means of the transverse field Ising model with nearest neighbor interaction. The 3D graphs plotted by the various physical parameters give a clear appreciation and qualitative understanding of the reentrant phase behavior of the system. Meanwhile the results show the close correlation between experimental phenomena and our theoretical calculation for the closed-loop behavior for the phase transition of the systems.

Key words: global phase diagram; reentrant behavior; transverse Ising model

P-4 Investigation of Ghanaian Natural Dyes for Possible Application in Dye Sensitized Solar Cells (Dsscs)

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Abstract

DSSCs provide a viable alternative to conventional silicon based solar cells due to their low cost of fabrication, easy to process, semi-transparent architecture, and environmental friendliness. However, the narrow absorption spectrum of current DSSCs devices leaves much room for improvement. And so, recent research works aim at broadening the absorption spectrum for efficient photon absorption and electricity generation. Amongst techniques explored are, the panchromatic (use of different dyes) and tandem (multi-layer device architecture) engineering of devices. Therefore, this work shall explore natural dyes or dye cocktails of Ghanaian origin with broad absorption spectrum for possible application in dye sensitized solar cells.

Keywords: Dye sensitized solar cells, natural dye, tandem structures, and panchromatic engineering.

P-5 Experimental and Computational Study of Transition Metal Doped Zinc Oxide

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Abstract

Pristine and transition metal (Fe, Mn, Co and Ni) doped ZnO powders were synthesised using a hydrothermal method and the crystalline phases characterised using x-ray powder diffraction. The band gap energies of the samples were measured using photoluminescence emission spectroscopy. Doping was done at concentrations of 1, 2, 4 and 8 mol %. Computational studies were carried out on undoped and transition metal (Fe, Mn, Co and Ni) doped ZnO using the Generalized Gradient Approximation (GGA) of the Density Functional Theory (DFT) implemented in Quantum ESPRESSO. Doping was done at concentrations of 5.56 atomic % and 11.11 atomic %. The computational results confirmed the trend observed experimentally, with the band gap energies increasing with doping. Mn – and Fe – doped ZnO showed the largest increase. The unit cell volume increased for Fe – and Mn – doping, in both the experimental and computational results. However, while the computational results predicted a narrowing in the unit cell volume for cobalt and nicked doping, the experimental results showed an increase for cobalt and a marginal increase for nickel.

P-6 Synthesis, Characterizations and Applications of Copper Nanoparticles

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Abstract

In recent times, copper nanoparticles have found different applications due to their unique optical, catalytic, mechanical and electrical properties. Copper plays an important role in electronic circuits because of its excellent electrical conductivity. Copper nanoparticles have also been used as catalysts with high efficiency due to its high surface area. It is a good alternative for noble metals such as silver and gold as it is highly conductive and more economical. In this research a novel green method was employed to synthesize copper nanoparticles using different plant extracts as capping agents. Moringa leaves extract, aloevera leaves extract were used as capping agents while ascorbic acid was used as antioxidant. The copper nanoparticles were synthesised by the reduction and precipitation of copper from copper sulphate solution. The synthesized nanoparticles were characterized by means of p-XRD, SEM, FTIR and UV spectroscopy. The IR spectra obtained indicated that the plant extracts were adsorbed (capped) on the surface of the copper nanoparticles through the functional groups present. The copper nanoparticles with Moringa extract exhibited blue luminescence under the UV light. The synthesised copper nanoparticles were further tested for antimicrobial properties and also used as catalysts in organic syntheses.

Keywords: copper nanoparticles, co-precipitation, green synthesis, moringa extract, aloevera leaves

P-7 Evaluation of the properties of some nontraditional vegetable oils from Northern Ghana.

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Abstract

The sources of traditional vegetable oils have been monopolized by a few plants to the neglect of other potential sources with comparable or enhanced properties. Ten neglected and underutilized vegetable oil seeds (Sesamum indicum (sesame), Lagenaria leucantha (calabash), Adansonia digitata (baobab), Ceiba pentandra (kapok), Balanites aegyptiaca (desert date), Hibiscus cannabinus (kenaf), Hibiscus sabdariffa (roselle), Trichosanthes kirilowii (sponge), Cucumeropsis edulis ('neri') and Cucurbita moschata (butternut squash)) were sampled from the northern part of Ghana. The oils were extracted with Soxhlet apparatus using n-hexane as solvent. Oil content of the samples ranged from 13.95 % to 52.91 %. Characterization of the oils was done using AOAC methods for physicochemical properties, FTIR analysis for the functionality and thermogravimetric analysis (TGA) for thermal decomposition profile. All the extracts were liquid at room temperature. The T. kirilowii seed oil presented distinct properties in colour, scent, acid value and FFA content. The FTIR spectra showed similar functional groups for all the ten samples in the diagnostic region, however, slight differences were noticed in the finger print region. TGA curves for the oils treated up to a temperature of 600°C indicated a twostep decomposition profile for all the samples. A. digitata seed oil was the most thermally stable, while *B. aegptiaca* seed oil gave the least residue after decomposition.

Key words: extraction, physicochemical, decomposition profile, FTIR, thermal stability.

P-8 Deposition of Zinc Chalcogenide Nanomaterials at the Water-Toluene Interface

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Abstract

Nanostructured thin films of ZnE (E=S, Se, Te) have been prepared at the toluene-water interface by reacting toluene solutions of alkyidithiocarbamates/ cupferronates with aqueous chalcogenide ions obtained by the borohydride reduction of sulphur, selenium and tellurium powder. The thin film deposits were characterized by powder X-ray crystallography p-XRD, scanning and transmission electron microscopy and absorption spectroscopy. The influence of deposition conditions such as precursor concentrations, temperature as well as deposition times were studied. The average crystallite sizes of the as-prepared nanoparticles at different temperatures, concentrations and deposition times ranged from 1.3 to 6.9 nm for ZnS, 2.0 to 7.1 nm for t-Se and 1.8 to 6.7 nm for t-Te. The dislocation densities ranged from 1.14 to 9.33×10^{17} lines/m for ZnS, 2.0 to 8.7 x 10^{17} lines/m for t-Se and 2.22 to 6.5×10^{17} lines/m for t-Te. The shape of the as-prepared nanoparticles at different temperatures was studied by SEM and gave morphologies from flowers to nanowires. The band gaps obtained for ZnS ranged from 3.6 to 3.88 eV, t-Se ranged from 2.86 to 3.91 eV and for t-Te from 3.6 to 3.9 eV.

P-9 Properties of Cu-Doped ZnS Thin Films Deposited from Acidic Chemical Baths

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Abstract

Zinc sulphide (ZnS) buffer layers are a wider energy band gap alternative to the cadmium sulphide (CdS) buffer layers currently used in copper indium gallium diselenide (CuInGaSe₂)-based solar cells. However extrinsic doping of the ZnS is important to lower the resistivity of the layers and to improve flexibility of device design. In this work, Cu-doped ZnS nanocrystalline films have been deposited on silica glass substrates from acidic chemical baths. The Cu- concentration was varied from 0 at. % to 40 at. %, keeping other deposition parameters constant. The as-deposited and annealed films were characterised by a variety of techniques. The X-ray diffraction data taken on these samples showed a broad peak corresponding to the (111) plane of cubic ZnS and also confirmed the presence of Cu. The annealed samples had well defined and more intense peaks indicating an improvement in crystallinity. The electrical conductivities of the films, measured by the four probe technique, showed an increase with increasing Cu-concentration. UV-Visible Optical Absorption measurements also showed variations in the optical transmittance with increasing Cu-concentration.

P-10 Quantum Mechanical Study of the Kinetics, Mechanisms and Thermodynamics of the Gas-Phase Decomposition of Pb[(ⁱPr)₂PSSe]₂ Single-Source Precursor

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Abstract

The reaction mechanism of the gas phase decomposition of Pb[(iPr)2PSSe]2 singlesource precursor has been investigated theoretically by means of the density functional theory (DFT). The geometries of all the stationary points and the selected points along the potential energy surfaces were optimized at the M06/LACVP* level of theory. The harmonic vibrational frequencies of all the stationary points were calculated at the above same level of theory. Ten possible reaction pathways including seventeen reaction pathways on both the singlet and doublet potential energy profiles were explored. The results indicate that the steps that lead to PbS formation on both the singlet and the doublet potential energy surfaces are favored kinetically over those that lead to PbSe and ternary PbSe_xS_{1-x} formation. However, thermodynamically, the steps that lead to ternary PbSexS_{1-x} formation are more favorable than those that lead to PbSe and PbS formation on the doublet PESs. Moreover, the energetics also suggests the proposed scheme involving the dissociation of PbSe to be the most stable species on the singlet PES. Density functional theory calculations of the gas phase decomposition of the complex indicate that the deposition of ternary PbSe_xS_{1-x} in chemical vapor deposition may involve more than one steps but the steps that lead to the its formation are consistent with a dominant role for thermodynamic factors, than kinetic.

PROFILES OF PLENARY SPEAKERS

DR. ESSSEL BEN HAGAN



Dr. Essel Ben Hagan holds a PhD in Mechanical Engineering (Energy Modelling and Policy) and he is Adjunct Associate Professor in the Department of Mechanical Engineering, Kwame Nkrumah University of Science and Technology, Kumasi. Dr. Hagan is a Consultant with over 25 years of experience in renewable energy policy and technologies. He has comprehensive understanding of the financial, legal, institutional and regulatory setup of power markets as well as sound experience in small-to medium scale renewable energy project development and financing in Africa. Dr. Hagan's consulting experience covers West, East and Southern Africa including Angola, Benin,

Cote d'Ivoire, Gambia, Ghana, Kenya, Liberia, Mali, Nigeria, Senegal, Sierra Leone, Swaziland, Tanzania and Zimbabwe. Dr. Hagan has considerable experience in working with development agencies and finance institutions, and his consulting clients include the World Bank, UNDP, UNEP, UN Economic Commission for Africa, African Development Bank, Danish Development Agency (DANIDA) and German Development Cooperation (GIZ). He has published several scientific papers on renewable energy in international journals and he is a co-author of a book entitled "Biomass Conversion and Technology" which is used as learning material under the UNESCO Energy Engineering Series.

DR. KWAME AMPOFO



Dr. Kwame Ampofo holds a PhD degree in Energy Management & Policy from the University of Pennsylvania (UPenn) in Philadelphia, USA (1993); an MSc degree in Chemical Engineering from the Mendeleev Institute of Chemical Technology, in Moscow, Russia (1982) and a BSc degree in Chemistry and Mathematics from the University of Ghana, Legon (1974). He also has formal training in a number renewable energy disciplines, including: "Renewable Energy Engineering" (Post-graduate Diploma) from

Sogesta College in Italy and "Rural Applications of Biogas Technology" (Diploma) from the Biogas Research & Training Center (BRTC) in Chengdu, China.

Dr. Ampofo has an extensive working experience, having worked in the Chemistry Department of the Institute of Industrial Research (IIR) of the Council for Scientific and Industrial Research (CSIR) of Ghana, as a Research Scientist for sixteen (16) years, heading the Energy Research Programme. Later, he was appointed a Commissioner at the Energy Commission of Ghana where he served in that capacity for four (4) years, from 1997 to 2001. In the year 2001, Dr. Ampofo entered the Parliament of Ghana as the Member of Parliament (MP) representing the South Dayi Constituency. During this period, he was appointed the Parliamentary Ranking Member on Mines and Energy by the Office of Parliament. He was later appointed the CEO of the Tema Oil Refinery (TOR) in 2009 and was re-assigned in 2010.

Dr. Kwame Ampofo is currently the Chairman of the Board of Directors of the Energy Commission of Ghana.



DR. HANNE LAURITZEN

Technical University of Denmark (DTU), Institute for Energy Conversion and Storage is internationally recognized for pioneering roll-to-roll processing of polymer solar cells, and for being uncompromised with respect to requiring stability, processability and scalability of any polymer solar cell concept worth investigating. DTU's effort on emerging solar cells

is headed by Professor Frederik C. Krebs. Dr. Hanne Lauritzen has been working closely with Professor Krebs for the last 7 years. Her key focus is technology strategy, technology transfer, and industrialization. Recently she has been heading a Danida sponsored Danish-Ghanaian project that finished June 2016. The objective of the project was to evaluate the feasibility of establishing a Ghanaian self-sustained business rooted in the polymer solar technology. Project partners were Kwame Nkrumah University of Science and Technology and Ashesi University College.

Before entering DTU, Dr. Lauritzen has held various positions in academia and industry. Her work has concerned all major PV technologies (crystalline silicon, inorganic thin film, dye-sensitized and organic PV), and she has been involved projects covering the entire value chain from materials via processing to product development, deployment and endof-use scenarios.

Hanne Lauritzen holds a PhD in solid state physics from University of Oslo, Norway (1989).



DR. P. JOHN THOMAS

Dr. P. John Thomas is currently a Lecturer of Physical Chemistry at School of Chemistry, Bangor University. His research is concerned with solid state chemistry including: synthesis and assembly of nanocrystals, charge transport in films of nanocrystals, interfacial phenomena and self-assembly. He is particularly interested in nanocrystalline architectures for energy generation applications. He has authored approximately 50 papers, a monograph on nanocrystals and contributed to a number of books and reports. He currently co-edits a Royal Society of Chemistry Book Series on Nanoscience.

He was a lectureship in Bangor in 2012. Previously, he was an RCUK research fellow at the University of Manchester. He obtained his Ph.D from JNCASR, Bangalore had been a post-doctoral fellow in Bangalore (with C.N.R. Rao and G.U. Kulkarni) and Manchester (with Paul O'Brien). He is a member of the Royal Society of Chemistry and a Fellow of the Higher Education Academy.

PROF. NEERISH REVAPRASADU



Prof. Neerish Revaprasadu is a professor of Chemistry and SARChI Chair holder in Nanotechnology at the University of Zululand, South Africa. He obtained his B,Sc(Hons.) from University of Natal in 1993 and Ph.D from Imperial College, London in 2000. He started as a Senior Lecturer at Unizulu in 2000 promoted to associate professor in 2004

and full professor in 2008. His research interest is in the synthesis and processing of semiconductor nanomaterials. He has published 150 articles in peer reviewed journals. He was elected Member of South African Academy of Science (ASSAF) in 2014.

PROF. PETER J SKABARA

James Young Chair of Chemistry

WestCHEM, Department of Pure and Applied Chemistry, University of Strathclyde

Education: BSC (Hons) 1991 (London) Bryce) PhD 1994 (Durham, Prof Martin



Professional Career:

1994-1995:	Postdoctoral researcher, Max-Planck Institute for Polymer Research, Mainz, with Klaus Müllen
1995-2000:	Lecturer, Sheffield Hallam University
2000-2005:	Senior Lecturer, University of Manchester
2005-present:	Professor, University of Strathclyde, Head of Department 2010-2013

Deputy Editor-in-Chief for Journal of Materials Chemistry C (from 2013)

Research Interests

- 1) Plastic electronics, device fabrication
- 2) Synthesis of electroactive materials, electrochemistry, spectroelectrochemistry
- 3) Self-assembly, non-covalent interactions, control of conformation

Published over 160 papers.

Honors

2005:	Leverhulme Trust Research Fellow
2006:	Visiting research scholar at the University of California, Los Angeles
2010:	Visiting research scholar at McGill University, Montreal
2013:	Visiting Professor at UPMC, Paris
2014:	Visiting Professor at Nagoya University, Japan
2014:	Royal Society Wolfson Research Merit Award

PROF. PAUL O'BRIEN CBE FRS FREng



Paul O'Brien is Professor of Inorganic Materials Chemistry in both the School of Chemistry and the School of Materials at University of Manchester. He was Research Dean 2000-02., Head of the School of Chemistry 2002-09 and Head of the School of Materials (2010-15). He founded Nanoco in 2001 now listed on LSE.

He graduated from Liverpool University in 1975, obtained his Ph.D. from the University of Wales, Cardiff in 1978 and was immediately appointed as a lecturer at Chelsea College, University of London. He moved to Queen Mary and Westfield College in 1984 and was promoted to a chair in 1994. In 1995 he moved to Imperial College and became the Sumitomo/STS Professor of Materials Chemistry (1997–2003). He was Regents appointed Visiting Professor at Georgia Institute of Technology (1996–1999). He is a Fellow of the: Royal Society of Chemistry (Chartered Chemist), Institute of Materials, Minerals and Mining (Chartered Engineer) Fellow of The Royal Society London (2015), IUPAAC, The Learned Society of Wales and the Royal Academy of Engineering (2016). He received the 2007 Kroll Medal from the IoM3, the first Peter Day Award for Materials Chemistry from the RSC in 2009 and The Longstaff Medal (2016). In 2006 he was awarded the first honorary D.Sc. degree of the University of Zululand, South Africa and holds honorary degrees from Liverpool (2013) Aveiro, Portugal (2015) and QMUL (2016).

As a fellow of the Royal Society of Chemistry he chaired the Materials Forum and was a member of the Council of the RSC 2003-12 and an inaugural Vice President (2010-12). He has lectured widely to the public, especially young people and received the Colin Humphries Award of the IoM3 for outreach activities in 2011 and their Platinum Medal (2014). In 2016 his work in Science and engineering was recognized by the award of a CBE.