

Middle East Doctoral Student Workshop on "Communicating the Chemical Sciences"

Amman, Jordan, Nov 9–15, 2009

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SCOPE OF THE WORKSHOP

The workshop precedes the conference "Frontiers of Chemical Sciences IV: Research and Education in the Middle East. A Bridge to Peace and International Development" (Malta IV, Chair: Z. M. Lerman) and will start at 6 pm on November 9, 2009. The main goal of the conference is to promote communication in and via Science among young scientists. Questions discussed: How is Science created, how do we communicate Science, how do we talk in public, to present own work to persons from different fields, to formulate the essence of own work, to summarize a talk and a discussion, to learn to ask questions, to find a proper form for criticism, to accept criticism, to enter a dialog. 15 advanced international doctoral students from the middle east and from Germany have been admitted to the school.

The workshop concentrates on student talks and discussions. Students are asked to bring a 10 min power–point presentation of their PhD project which they present in the "1st presentation". The other students are asked to comment the presentation. The presenter's task later is to improve and to shorten the presentation to about 8 min, highlighting the essential ideas. In the next session the student will present the improved version. On the final day, the talks will then be presented in the afternoon of Nov. 14, in front of some participants of Malta IV. Each session will start with talks from senior Scientists. For Thursday, November 12, an excursion to Petra, Jordan is planned.

WORKSHOP PROGRAM

MONDAY Nov 9

Until 17:00	Arrival. For those coming earlier: recommended individual visit of citadel (10-16h) (app. 5 km walking distance from Hotel), downtown Amman and/or Abu-Darwish Moschee
17:00	Mixer
17:45	Departure to Al-Hussein Cultural Center (Ras Al Ein) (by taxi) 20th Anniversary of the Fall of the Berlin Wall
18:30	Evening Reception by the The Ambassador of the Federal Republic of Germany, Dr. Joachim Heidorn, and Mrs. Anna-Maria Werner-Heidorn (not public, all participants are invited. Invitation provided before departure needs to be shown at the entrance
19:30	Jordanian and German National Anthems Welcome speech by H.E. the German Ambassador
19.45	Documentary film: " How the Wall came down... "
20.15	Jordanian special guest band
21.00	German band "17 Hippies" The concerts are part of the "European Film Festival" and are presented with the French Cultural Center in collaboration with the Swedish EU Presidency. With the generous support of the Delegation of the European Commission Amman.
App 22:30	Return to hotel (by taxi)

TUESDAY Nov 10

7:30 – 8:30	Breakfast
9:00 – 9:30	OPENING OF THE WORKSHOP Hans-Heinrich Limbach (Berlin) "How to communicate in Science?"
9:30 – 12:30	SESSION 1 Discussion Leader: Monique Chan Huot , Berlin, Germany
9:30 – 9:40	Almas Haider , Braunschweig, Germany "Clean Development Mechanism - Opportunities in the Capital of India in the Sector of Municipal Solid Waste Management"
9:40 – 10:30	Discussion
10:30 – 11:00	Coffee Break
11:00 – 11:10	Mohamed Hammouda , Mansoura University, Egypt "Study on the chemistry of 2-acetyl-1,3-indandione"
11.10 – 12:00	Discussion
12:00 – 12:10	Merve Gürtekin , Marmara Research Center, Turkey "UV curable hybrid materials for direct methanol fuel cells"
12:10 – 13:00	Discussion
13:00 – 14:00	Lunch
14:00 – 16:00	SESSION 2 Discussion Leader: Stepan Lesnichin , Berlin, Germany
14:00 – 14:10	Mohammad Al-Zoubi , Al-Karak, Jordan "Removal of Chromium from Industrial Effluents by Sand Filtration"
14:10 – 15:00	Discussion

15:00 – 15:10	Louaiy Albaqaien , Al-Karak, Jordan "Properties of Semiconductors"
15:10 – 16:00	Discussion
16:00 – 16:30	Coffee break
16:30 – 18:30	SESSION 3 Discussion Leader: Alexandra Lauer , Berlin, Germany
16:30 – 16:40	Ceyda Koyuncu , Marmara Research Center, Turkey "Effects of Cr, Zn and Ag Dopants on the Photocatalytic Properties of TiO ₂ "
16:40 – 17:30	Discussion
17:30 – 17:40	Moteaa El-Defdar , Cairo, Egypt "Microwave-Assisted Palladium Catalyzed Organic Synthesis"
17:40 – 18:30	Discussion
18:30 – 19:30	Dinner
20:00 – 21:30	SESSION 4 Discussion Leader: Salih AlJabour , Jerusalem, Palestine and Berlin, Germany
20:00 – 21:00	Henning Hopf (Braunschweig, Germany) "Can Invention be invented?"
21:00 – 21:30	Discussion

WEDNESDAY Nov 11

7:30 – 8:30	Breakfast
9:00– 11:00	SESSION 5 Discussion Leader: Mohammad AlZoubi , Al-Karak, Jordan
9:00 – 9:10	Khalil Hamza , Jerusalem, Israel "Heterogenization of reagents and catalysts by modern methods. Application of the heterogenized materials to multi-step one-pot reactions"
9:10 – 10:00	Discussion
10:00 – 10:10	Haneen Daoud , Al-Karak, Jordan "Self- Assembly in the Synthesis of 2D Supramolecular Coordination Polymers"
10.10 – 11:00	Discussion
11:00 – 11:30	Coffee Break
11:30– 15:00	SESSION 6 Discussion Leader: Khalil Hamza , Jerusalem, Israel
11:30 – 11:40	Alexandra Lauer , Berlin, Germany "Photoinduced Reactions and Ultrafast Dynamics of Anthracene-9,10-endoperoxide"
11:40 – 12:30	Discussion
12:30 – 13:30	Lunch
14:00 – 14:10	Salih AlJabour , Jerusalem, Palestine and Berlin, Germany "Photochemistry Study of Cyclopenta-2,4-dienimine"
14:10 – 15:00	Discussion
15:00 – 17:00	SESSION 7 Discussion Leader: Meggie Hakim , Haifa, Israel
15:00 – 15:10	Stepan Lesnichin , Berlin, Germany "Investigation of the active site structure and properties of carbonic anhydrase by NMR spectroscopy "
15:10 – 16:00	Discussion

16:00 – 16:10	Meggie Hakim , Haifa, Israel "NaNose for Early Detection of Lung Cancer via Breath Samples"
16:10 – 17:00	Discussion
17:00 – 17:30	Coffee break
17:30 – 19:30	SESSION 8 Discussion Leader: Merve Gürtekin , Marmara Research Center, Turkey
17:30 – 17:40	Julia Mahamid , Rehovot, Israel "Mapping of Amorphous Calcium Phosphate Transformation into Crystalline Mineral in the Fin Bones of Zebrafish: From the Cell to the Bone"
17:40 – 18:30	Discussion
18:30 – 18:40	Monique Chan Huot , Berlin, Germany "NMR studies of model system of PLP dependent enzymes"
18:40 – 19:30	Discussion
19:30	Dinner

THURSDAY Nov 12

6:00 – 22:00 **Excursion to Petra**

Friday Nov 13

7:30 – 8:30	Breakfast
9:00 – 10:30	SESSION 9 Discussion Leader: Julia Mahamid , Rehovot, Israel Helmut Ringsdorf (Mainz, Germany) "Tumor Research for Beginners by Biological Rational for the Development of Polymeric Antitumor Agents"
9:00 – 10:00	
10:00 – 10:30	Discussion
10:30 – 14:00	Individual Work of Doctoral Students on their Presentation
10:30 – 11:00	Coffee break
12:30 – 13:00	Lunch
14:00 – 14:40	Session 10 Rehearsal 1 Discussion Leader: Moteaa El-Deftar , Cairo, Egypt Almas Haider , Braunschweig, Germany Mohamed Hammouda , Mansoura University, Egypt Merve Gürtekin , Marmara Research Center, Turkey Louaiy Albaqaien , Al-Karak, Jordan
14:40 – 15:20	Session 11 Rehearsal 2 Discussion Leader: Mohamed Hammouda , Mansoura University, Egypt Mohammad AlZoubi , Al-Karak, Jordan Ceyda Koyuncu , Marmara Research Center, Turkey Moteaa El-Deftar , Cairo, Egypt Khalil Hamza , Jerusalem, Israel
15:20 – 15:40	Coffee Break
15:40 – 16:20	Session 12 Rehearsal 3 Discussion Leader: Almas Haider , Braunschweig, Germany Haneen Daoud , Al-Karak, Jordan Alexandra Lauer , Berlin, Germany

Salih AlJabour, Jerusalem, Palestine and Berlin, Germany
Stepan Lesnichin, Berlin, Germany

16:20 – 17:00

Session 13 Rehearsal 4

Discussion Leader: **Louaiy Albaqaien**, Al-Karak, Jordan
Meggie Hakim, Haifa, Israel
Julia Mahamid, Rehovot, Israel
Monique Chan Huot, Berlin, Germany

17:00

Visits of Amman with Dinner

SATURDAY Nov 14

7:30 – 8:30

Breakfast

9:00 – 12:30

SESSION 14

Discussion Leader: **Haneen Daoud**, Al-Karak, Jordan

9:00 – 10:00

Ziad Salem Abu-Hamattah (Al-Balqa' Applied University, Jordan)
 "Water Resources and Environmental Management in Jordan and the Middle East"

10:00 – 10:30

Discussion

10.30 – 11:00

Coffee Break

11:00 – 12:30

SESSION 15

Discussion Leader: **Ceyda Koyuncu**, Marmara Research Center, Turkey

11:00 – 12:00

Catherine E. Costello (Boston, USA)
 "Mass Spectrometry-Based Methods for Proteomics"

12:00 – 12:30

Discussion

12:30 – 13:30

Lunch

14:00 – 17:00

Student Presentations at Malta IV

14:00 – 14:40

Session 1

Discussion Leader: **Moteaa El-Deftar**, Cairo, Egypt

14:00 – 14:10

Almas Haider, Braunschweig, Germany
 "Clean Development Mechanism - Opportunities in the Capital of India in the Sector of Municipal Solid Waste Management"

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 "Heterogenization of reagents and catalysts by modern methods. Application of the heterogenized materials to multi-step one-pot reactions"

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Coffee Break

15:50 – 16:30

Session 3

Discussion Leader: **Almas Haider**, Braunschweig, Germany

15:50 – 16:00	Haneen Daoud , Al-Karak, Jordan "Self- Assembly in the Synthesis of 2D Supramolecular Coordination Polymers"
16:00 – 16:10	Alexandra Lauer , Berlin, Germany "Photoinduced Reactions and Ultrafast Dynamics of Anthracene-9,10-endoperoxide"
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16:20 – 16:30	Stepan Lesnichin , Berlin, Germany "Investigation of the active site structure and properties of carbonic anhydrase by NMR spectroscopy "
16:30 – 17:00	Session 4 Discussion Leader: Louaiy Albaqaien , Al-Karak, Jordan
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16:40 – 16:50	Julia Mahamid , Rehovot, Israel "Mapping of Amorphous Calcium Phosphate Transformation into Crystalline Mineral in the Fin Bones of Zebrafish: From the Cell to the Bone"
16:50 – 17:00	Monique Chan Huot , Berlin, Germany "NMR studies of model system of PLP dependent enzymes"
19:00 – 20:45	Welcome Reception Malta IV, including Dinner at the Caballeros Restaurant, Kempinski hotel
21:00 – 22:00	Plenary Session: Discussion Leader: Hannah Hallak, Bethlehem University (Palestinian Authority) "Advances in atomic physics. An overview" Claude Cohen-Tannoudji, École Normale Supérieure (France)
22:00	Informational discussions

SUNDAY Nov 15

7:30 – 8:30	Breakfast
9:00	Departure

WORKSHOP PARTICIPANTS

Doctoral students

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Lecture

Can invention be invented?

Henning Hopf

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Since our technical civilization – in fact: our survival – depends on constant innovation the question has often been asked whether the process of invention can be planned itself and be subjected to the scientific method.

The aim of the lecture is to show (by taking ground-breaking innovations from chemistry, physics and some other areas) that as an act of creativity/creation invention *cannot* be planned but is largely an irrational, accidental, and very subjective process. However, there are certain conditions that favor and/or disfavor invention. These factors will be discussed as well as a pragmatic approach (heuristics)^[1] to improve ones own performance to become a good/better researcher.

- [1] N. Graulich, P. R. Schreiner, H. Hopf, *Chem. Soc. Reviews*, **2010**, *in press*. *Heuristics make a chemist smart.*

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Lecture

Tumor Research for Beginners by Biological Rational for the Development of Polymeric Antitumor Agents

Helmut Ringsdorf

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Today some of the most exciting research in the world is being undertaken in the field of molecular biology and medicine. Many challenges exist in identifying disease at the earliest possible stage and attempts to develop concepts to prevent and treat life threatening illnesses, e.g. like cancer on a biomedical rational. In Europe and USA approximately one in three people get some form of cancer; of these patients one in four die of their diseases. How can we cope with it? What can we learn from Mother Nature? Nowadays, many primary tumors – early recognized - are treatable and can even be cured. So, where is the problem?

The problems are the metastases: Most cancer death are based on metastases induced secondary tumors. Starting from singled out tumor cells, vascularisation (angiogenesis) is needed to support these tumor nodules with oxygene, nutrition etc. Developing their growing vascularisation systems hastily, the tumors make mistakes leading to hyperpermeable arteries and veins by the formation of irregularities and even holes in their blood vessels. These defects open new opportunities for tissue and cell selective localization of nanoscale drug delivery systems, which after i.v.-injection can not leave the perfect arteries and veins in healthy tissue. Based on this concept applying polymer therapeutic has led to new dimensions in tumor chemotherapy [1-4] and tumor targeting. Polymer antitumor agents and polymeric angiogenesis inhibitors are not only in clinical Phase I- and Phase II-studies, but several polymer therapeutics are already in clinical used.

- [1] Duncan, R.: The Dawning Era of Polymer Therapeutics. *Nature Reviews* 2, 347 (2003).
- [2] Gros, L., Ringsdorf, H., Schupp, H.: Polymeric Antitumor Agents on a Molecular and on a Cellular Level? *Angew. Chem. Int. Ed. Engl.*, 20, 305 (1981).
- [3] “Polymer Drugs in the Clinical State. Advantages and Prospects.” *Adv. In Exp. Medicine and Biology*, Vol. 519 (2003), edited by Maeda, H., Kabanov, A., Kataoka, K., Okano, T.
- [4] Satchi-Fainaro, R., Puder, M., Folkman, J. et. al.: “Targeting angiogenesis with conjugate of HPM copolymer and TNP-470”, *Nature Medicine*, 10, 255 (2004).

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Lecture

Water Resources and Environmental Management in Jordan and the Middle East

Ziad Salem Abu-Hamattah

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Jordan is one of the arid and semi arid regions where 90% of the country receives less than 200 mm of annual rainfall. The Area of Jordan is about 90,000 km² and 6 million inhabitations in the year 2008. The water quality is of increasing concern due to the limited water resources and their vulnerability to sewerage and industrial waste contamination and over abstraction and mining of aquifers [1].

Jordan suffers from scarcity of available sources of water and relies on rainwater to replenish surface water and groundwater alike. The increasing population in addition to the economic and agricultural growth led to an increasing demand for water. The water supply to various sectors has risen from 801.44 million cubic meters in 1999 to 925.2 million cubic meters in 2006 [2]. The inability to provide non-traditional water sources has increased pressure on traditional sources to meet the rising demand for water.

The issue of water resources in the Middle East is of prime importance for peace and for the development of the region in the future [3]. In this talk, current problems are reviewed and research efforts described designed to tackle this problem [4].

[1] World vision report.

[2] Pressure on water supply in various sectors The Hashemite Kingdom of Jordan
Department of Statistics, Global Water Day Date: 23. Mar . 2008.

[3] http://www.un.org/Depts/dhl/me_water.htm.

[4] Environ. Sci. Technol., 2009, 43 (6), pp 1769–1775.

Lecture

Mass Spectrometry-Based Methods for Proteomics

Catherine E. Costello, Giuseppe Infusini, Weiwei Tong, Vivek Bhatia, Weidong Cui, Liang Han, Yan Jiang, Lei Li, David H. Perlman, Krystyn B. Ross, Roger Théberge, Yan Wang, Cheng Lin, Mark E. McComb

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Full coverage of proteomes requires not only identification and quantification of proteins that indicate which cellular pathways are affected under the conditions chosen for study, but also characterization of post-translational modifications (PTMs) to these proteins [1]. Antibody-based pull-down methods retrieve molecular complexes whose composition can vary depending on the presence of sequence elements or PTMs of key proteins [2]. Alternatively, chemical modifications to specific amino acids (*e.g.*, ICAT, fluorolabels) or isolation methods that are based on chemical interactions (*e.g.*, with phosphate groups) enable the enrichment of proteins/peptides that bear specific markers for processes such as oxidative stress or cancer [3-5]. We have developed strategies for separation of intact proteins or peptides and for determination of their complete amino acid sequences and the identification and site-specific localization of PTMs. If the PTMs are labile under routine MS conditions (*e.g.*, phosphorylation, sulfonation, glycosylation), particular attention needs to be paid to the selection of dissociation conditions that preserve and, ultimately, fully define the modification(s). When individual proteins have multiple PTMs, only analysis of the intact proteins will provide information on the correlations between PTMs. Isolated proteins may be subjected to proteolytic or chemical degradation or analyzed in their intact form (top-down proteomics). Examples from recent and ongoing projects will be presented to illustrate some of the proteomic and glycomic strategies developed and utilized in our Center.

Acknowledgements: This research is supported by the National Institutes of Health, grant Nos. P41 RR10888, S10 RR15942, S10 RR020946, S10 RR025082 and contract No. N01 HV028178

- [1] F. Lavatelli, D. H. Perlman, B. Spencer, T. Prokaeva, M. E. McComb, R. Théberge, L. H. Connors, V. Bellotti, D. C. Seldin, G. Merlini, M. Skinner, C. E. Costello, *Mol. Cell. Proteomics* **2008**, 7, 1570-1583.
- [2] Y. Wang, A. B. Meriin, N. Zaarur, N. V. Romanova, Y. O. Chernoff, C. E. Costello, M. Y. Sherman, *FASEB Journal*, **2009**, 23, 451-463.
- [3] M. Sethuraman, M. E. McComb, H. Huang, S. Huang, T. Heibeck, C. E. Costello, R. A. Cohen, *J. Proteome Res.*, **2004** 3, 1228-1233.
- [4] W. Ying, D. H. Perlman, L. Li, R. Théberge, C. E. Costello, M. E. McComb, *Rapid Commun. Mass Spectrom.* In press
- [5] D. H. Perlman, H. Ashrafiyan, S. Bauer, N. S. Bryan, M. F. Garcia-Saura, C. C. Lim, B. O. Fernandez, M. E. McComb, C. E. Costello, M. Feelisch, *Circ. Res.*, **2009**, 104, 796-804.

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Student Talk

Clean Development Mechanism - Opportunities in the capital of India in the sector of Municipal Solid Waste Management

Almas Haider, Klaus Fricke

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Delhi is the most densely populated and urbanized city of India. The annual growth rate in population during the last decade (1991–2001) was 3.85%, almost double the national average. Delhi is also a commercial hub, providing employment opportunities and accelerating the pace of urbanization, resulting in a corresponding increase in municipal solid waste (MSW) generation. Presently the inhabitants of Delhi generate about 7000 tonnes/day of MSW, which is projected to rise to 17,000–25,000 tonnes/day by the year 2021. MSW management has remained one of the most neglected areas of the municipal system in Delhi. About 70–80% of generated MSW is collected and the rest remains unattended on streets or in small open dumps. Only 9% of the collected MSW is treated through composting, the only treatment option, and rest is disposed in uncontrolled open landfills at the outskirts of the city. The existing composting plants are unable to operate to their intended treatment capacity due to several operational problems. Therefore, along with residue from the composting process, the majority of MSW is disposed in landfills. In absence of leachate and landfill gas collection systems, these landfills are a major source of groundwater contamination and air pollution. On the same side Delhi is currently facing the problem of energy deficit, which is met by the combination of dynamic power shedding and power purchase from various independent power plants (IPP). As a project activity, in order to reduce the GHG emissions and to meet the energy requirement it has been proposed to convert MSW of Delhi into energy by the implementation of 7 project activities in different phases under Program of Activities (PoA). During PoA, an initiative will be launched to reduce GHG emissions and to increase the amount of available energy in the city and also improve the cash flow.

- [1] Gorai Landfill closure and Gas Capture Project, Mumbai, India, <http://cdmbazaar.com>
- [2] UNEP Risoe CDM/JI pipeline analysis and database. <http://www.cdmpipeline.org>
- [3] UNFCCC (2009), CDM Project Activities; <http://cdm.unfccc.int/ProgramOfActivities/index.html>
- [4] UNFCCC (2009), CDM Project Activities; <http://cdm.unfccc.int>

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Student Talk

Study on the Chemistry of 2-Acetyl-1,3-indandione

Mohamed El-Metwally Hamouda, E.M. Afsah, A.A. Fadda and S. Bondock

Chemistry Department, Faculty of Science, Mansoura University, Mansoura, Egypt, Email: mohamedhamouda83@yahoo.com

1,3-Indanedione and its derivatives showed a wide range of biological properties. Over twenty biological activities of 1,3-indanediones have been described, most are 2-substituted-1,3-Indanediones.

On the other hand, ketonic Mannich bases are important synthetic intermediates with a wide variety of applications, and also possess considerable pharmaceutical interest. The ketonic Mannich bases and related compounds are of synthetic relevance, and are promising as biologically active compounds.

The aim of the present work is to study the possible synthesis of some new ketonic Mannich bases related to 1,3-indanedione, and their conversion into some new heterocyclic systems of alkaloidal nature.

As a part of this study the alkylation of amines, thiols and active methylene compounds with ketonic Mannich bases will be investigated as a possible route to some new compounds of pharmaceutical interest related to 1,3-indanedione. Structure elucidation of the new compounds using, IR(Infrared), UV(Ultraviolet), ¹H-NMR(Proton nuclear magnetic resonance), C-13 and MS (Mass spectra) will be undertaken. The newly synthesized compounds will be tested as antimicrobial, antifungal and anticancer agents.

We thank the Chemistry Department, Faculty of Science, Mansoura University, Egypt, for the financial support, the German Academy Exchange Service (DAAD), the Free University of Berlin, and the Fonds of the Chemical Industry, Frankfurt. For giving me the chance to attend this conference.

- [1] V. Enchev, G. Ivanova, G. Pavlovic, M. Rogojerov, A. Ahmedova, M. Mitewa, *Journal of Molecular Structure* **2003**, 654, 1-3.
- [2] T. Zimmermann, *Journal of Heterocyclic Chemistry* **2000**, 37, 1571-1574.
- [3] M. Hammouda, M. A. Metwally, Z. M. Abou-Zeid, T. Zimaity, *Indian Journal of Chemistry*, **1999**, 32B, 440-444.

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Student Talk

UV curable hybrid materials for direct methanol fuel cells

Merve Gürtekin, Tülay Yılmaz İnan, Nilhan Kayaman Apohan

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A proton exchange membrane fuel cell transforms the chemical energy liberated during the electrochemical reaction of hydrogen and oxygen to electrical energy. The most commonly used membrane is Nafion[®] by DoPont[®]. Although Nafion has excellent chemical and mechanical stability, high proton conductivity, it has some disadvantages that restrict its industrial applications such as high cost and high methanol permeability. Therefore, lower cost polymers with high performance are strongly desired as alternative materials.

The hybrid formulations were polymerized under UV irradiation and, the gel percentage and swelling ratio of the membranes were calculated. The polymerization conversion of the organic part was investigated using photo-DSC. The structural characterization of the UV-cured hybrid membrane was performed by employing solid-state ²⁹Si-NMR spectroscopy. The results indicated that partial condensation was achieved. The thermal stabilities of the UV-cured nanocomposites were investigated by thermogravimetric analysis (TGA). The morphology of the hybrid materials was examined by scanning electron microscopy. In addition proton conductivity, methanol selectivity measurements were performed.

Fuel cells have emerged as an alternative power source because of their high-energy conversion efficiency and eco-friendliness. Among the various types of fuel cells, the direct methanol fuel cells (DMFC), where liquid methanol is used directly as the fuel, has the added advantages of safer handling and storage of the fuel, and a simpler overall system design [2]. Nafion at present is one of the most advanced commercially available membranes for DMFC. Although Nafion has excellent chemical and mechanical stability and high proton conductivity, it has some disadvantages that restrict its industrial applications such as high cost and high methanol cross-over. Therefore, lower cost membranes with high performance are strongly desired.

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Book of Abstracts

Student Talk

Removal of Chromium from Industrial Effluents by Sand Filtration

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This paper is concerned with a cost-effective approach of removing a heavy metal, Chromium, from its aqueous solution by sand filtration. Solutions of varying chromium concentrations (50-250ppm) were prepared and passed through a column of sand. Effluent samples collected at different column depths were analyzed for the concentration of Chromium ions using an Atomic Absorption Spectrometer.

The injection rate and pH of the influent solution were also varied to study their effects on the Chromium removal efficiency of sand. A series of curves were constructed to determine the capacity of sand column at various depths. The removal efficiency was found to be in the range 89-100%. These high removal efficiencies were likely attributed to the strong affinity of chromium ions to the surface of sand particles.

It can be concluded that due to their nominal cost and relatively high adsorption capability, sand has the potential to be utilized for the cost-effective removal of heavy metals from water and wastewater.

Book of Abstracts

Student Talk

Properties of Semiconductors

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Semiconductor materials were studied in laboratories as early as 1830. The first materials studied were group of elements and compounds that were usually poor conductors if heated. Shining light on some of them would generate an electrical current that could pass through them in one direction only.

By 1874, electricity was being used not only to carry power, but to carry information. The telegraph, telephone, and later the radio were the earliest devices in an industry that would eventually be called electronics.

A semiconductor is a solid whose electrical conductivity is in between that of a metal and that of an insulator, and can be controlled over a wide range; either permanently or dynamically Semiconductors are tremendously important technologically and economically. Silicon is the most commercially important semiconductor, though dozens of others are important as well. Semiconductor devices, electronic components made of semiconductor materials, are essential in modern electrical devices, from computers to cellular phones to digital audio players.

Book of Abstracts

Student Talk

Effects of Cr, Zn and Ag Dopants on the Photocatalytic Properties of TiO₂

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Because of its high photocatalytic activity, TiO₂ has been studied extensively. When irradiated with UV light TiO₂ can decompose organic contaminants. However the wide band gap of TiO₂ limits the usage of visible light as a light source for photocatalysis [1]. Several studies have been carried out to develop the visible light activity of TiO₂ and it is demonstrated that metal ion doping is an effective way to enhance the photocatalytic activity of TiO₂ [2-4].

In this study photocatalytic TiO₂ powders and coatings will be prepared by sol-gel technique, using alkoxide solutions and effects of Cr, Zn and Ag dopants on the UV and daylight photocatalytic activity of TiO₂ will be investigated.

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Book of Abstracts

Student Talk

Microwave-Assisted Palladium Catalyzed Organic Synthesis

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Suzuki-Miyaura and Heck-Mizoroki C-C cross-coupling reactions of aryl and heteroaryl halides with various arylboronic acids and olefins were investigated using the catalytically active benzimidazole-based Pd(II)-precatalyst both under thermal as well as microwave irradiating conditions in water. The factors affecting the optimization of such reactions are investigated.

Sponsored by the Chemistry Department, Faculty of Science, Cairo University

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Student Talk

Heterogenization of reagents and catalysts by modern methods. Application of the heterogenized materials to multi-step one-pot reactions

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Many organic reactions can be carried out successfully only in the presence of catalysts. Most often, the catalyst is dissolved together with the reactants in an organic solvent or water. The separation of the products from the catalyst and reuse of the latter may constitute major problems. Therefore, in this work catalysts have been immobilized during sol-gel processes in porous solids and the reaction carried out in the pores. Examples [1-6] of various one-pot reactions will be presented.

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Student Talk

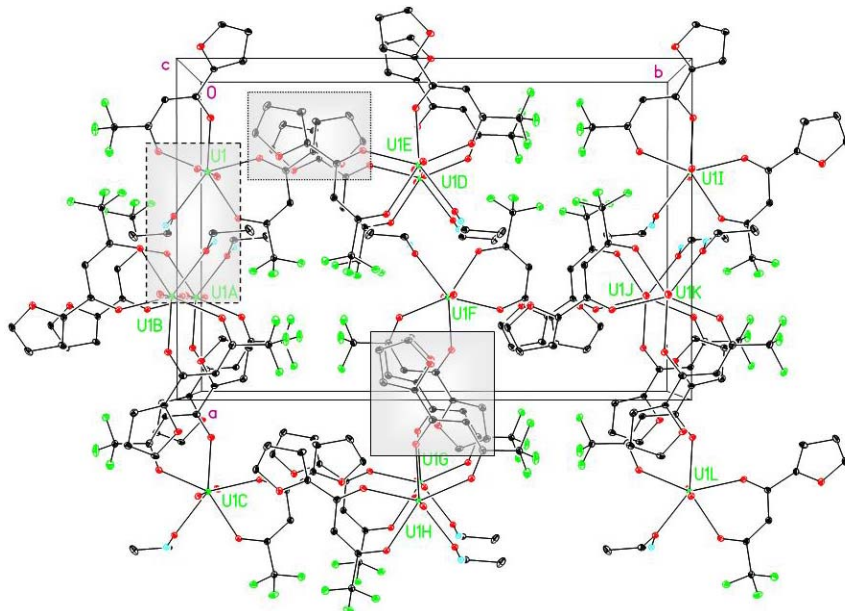
Self-Assembly in the Synthesis of 2D-Supramolecular Coordination Polymers

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2D-Supramolecules and supramolecular coordination polymers with the general formula $[M(L)_2 \cdot 2H_2O]$ and $[M(L)_2 \cdot (bpy)]_n$ (where M: Co(II), Zn(II), Cu(II), Fe(II), Mn(II), Ni(II), and UO₂; L = 3-benzoyl-1,1,1-trifluoroacetone (Htba) or 4,4,4-trifluoro-1-(2-furyl)-1,3-butanedione (Htfa); bpy = 4,4'-bipyridine) have been prepared by the direct self-assembly method. The solid-state structure for $[UO_2(tfa)_2]$ is discussed. The structures show a presence of non-covalent intermolecular interaction in the crystal structures. The magnetic, electronic and thermal properties are studied. The study is going to use these types of compounds in the separation and adsorption processes.



Book of Abstracts

Student Talk

Photoinduced Reactions and Ultrafast Dynamics of Anthracene-9,10-endoperoxide

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Anthracene-9,10-endoperoxide (APO) undergoes two different photoinduced reactions depending on the excitation wavelength: Cycloreversion, resulting in anthracene (AC) and singlet oxygen ($^1\text{O}_2$), and homolytic cleavage of the peroxide bridge, initially generating a biradical. Eventually this intermediate produces a diepoxide and other rearrangement products like anthraquinone (AQ). Room-temperature thermolysis of APO only produces AQ.

The electronic excited states of APO giving rise to the different reaction channels were characterized using femtosecond polarization resolved UV/IR pump-probe, and steady-state emission experiments, together with theoretical calculations [1].

The wavelength dependence of the photochemistry of APO was quantitatively investigated by absorption and ^1H NMR spectroscopy. The absolute photoreaction quantum yields of the primary and secondary products were determined for excitation wavelengths from 240 to 450 nm [2].

The ultrafast photoreaction dynamics of APO were investigated using femtosecond UV pump - supercontinuum probe spectroscopy. Excitation at 282 nm activates both reaction channels, but signals of different product contributions are separated in the analysis. Time constants for photoreaction and vibrational cooling processes are deduced from the transient absorption data [3].

Acknowledgements. Transient absorption measurements were done in cooperation with Dr. S. A. Kovalenko in the laboratory of Prof. N. P. Ernsting, Humboldt Universität zu Berlin. Financial support by Deutsche Forschungsgemeinschaft (DFG, project SFB450 TP B9) is gratefully acknowledged.

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Student Talk

Photochemistry Study of Cyclopenta-2,4-dienimine

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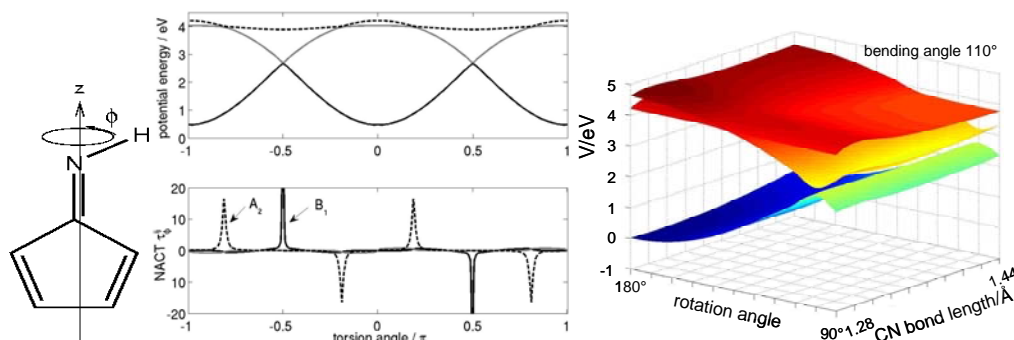
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Photochemical reactions which proceed via conical intersection are currently studied intensively since many fundamental process such as photosynthesis and the process of vision are triggered by such reactions [1,2]. Internal conversions, such as S1→S0 are of major importance in Photochemical reactions. These non-adiabatic processes proceed on typical time scales from a few tens of femto seconds to picoseconds [3]. The diversity of fascinating biological motors, such as the kinesin or myosin linear and ATP-ase rotary motor systems, has been a source of inspiration for development of artificial molecular mechanic devices such as switches, shuttles and muscles. Unidirectional rotation is achieved by a combination of a photochemically mediated cis-trans isomerization followed by an irreversible thermal isomerization [3].

The aim of studying cyclopenta-2,4-dienimine PES is to help in predicting and simulating photo-induced isomerization reaction in the presence of a conical intersection and finally design laser pulses for the control of the reaction. In cyclopenta-2,4-dienimine, such reactions are governed by a conical intersection between the ground and the first excited electronic state. A conical intersection is predicted on the basis of the Longuet-Higgins phase change rule as shown in several papers [5]. An important step towards the design of laser pulses for the control of torsional switches is the evaluation of the relevant non-adiabatic coupling terms (NACTs) which may induce the transition from the photo-excited reactant to the product. Prominent effects are expected near conical intersections or crossing seams. We predict that these should have symmetry properties according to the molecular symmetry group. The general rules for the symmetry properties of the NACTs may be used in order to assign their signs and nodal properties, which in turn may serve to test quantum chemistry calculations of the NACTs.



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Book of Abstracts

Student Talk

Investigation of the active site structure and properties of carbonic anhydrase by NMR spectroscopy

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Carbonic anhydrase (CA) is a widely occurring Zn metalloenzyme found in animal, plants and certain bacteria. In addition to its physiological important function, CA has been a topic of great interest since its activity as catalyst with a turnover rate of about 10^6 reactions per second (25°C) is among the highest for any known enzyme [1].

The catalytic activity of CA connects with the possibility of the facile proton shuttle between the metal ion and imidazol of histidine trough the bound water. Characterization of the H-bond network structure is greatly important for understanding the physiochemical and biological functions of the CA [2]. One of the best methods suitable methods suitable for such investigation is NMR spectroscopy.

However, as a result of the poor spectroscopic properties associates with the Zn-ion, it is a nontrivial issue to determine the structure of the active site of zinc enzyme by NMR directly. In this case are often used Co(II)-substituted models of enzymes. Owing to the similarities of the coordination chemistry of zinc (II) and cobalt (II), cobalt (II)-substituted enzymes retain all or partly of the active site of the native proteins and represent ideal model of the systems. Thus, studying structure of cobalt (II)-substituted enzymes by means NMR spectroscopy can be successfully applied, because Co(II) as a paramagnetic can induce hyperfine shifts on nuclei, for instance nitrogen, belonging to residues in the active site.

The useful information about the chemical properties of the active site of CA can be obtained by studying of suitable models that mimic the coordination environment of CA active site. The use of such models allows us to investigate the behavior of the ZnOH group in well defined environment by NMR spectroscopy in solution. Among several model compounds the most appropriate in our opinion are the $\text{Tp}^{\text{R}1,\text{R}2}\text{Zn-OH}$ complexes of Vahrenkamp *et al* [3].

In the present work we are trying to describe on the one hand the active site structure of the Co(II)-substituted enzyme by means solid state ^{15}N -NMR spectroscopy. On the other hand the chemical properties of model compounds by NMR spectroscopy in polar solvent at low temperature.

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Book of Abstracts

Student Talk

NaNose for Early Detection of Lung Cancer via Breath Samples

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Recent statistics have estimated that there were nearly 3 million new cases of cancer diagnosed in 2004 and over 1.7 million deaths from cancer in Europe and the USA, with lung cancer listed as one of the most common forms of cancer diagnosed and a leading cause of death.^{1,2} Conventional diagnostic methods for lung cancer occasionally miss tumors and they are costly and unsuitable for widespread screening. In contrast, breath testing, which links specific volatile organic compounds (VOCs) in exhaled breath to lung cancer conditions, is a fast, non-invasive diagnostic method. Studies of gas-chromatography/mass-spectroscopy (GC-MS) linked with a pre-concentrator have shown that several VOCs in breath appear to be elevated in instances of lung cancer.³⁻⁵ The compounds of interest are generally found in healthy human breath, but can be seen in distinctive mixture compositions and at elevated levels in the breath of diseased patients.

The overarching goal of this study is to compare the signatures and compositions of exhaled VOCs in lung cancer patients before surgery and after surgical removal of tumour. In the same context, the current study aims to better understand the pathophysiological meaning of exhaled VOCs and to determine whether they result from the tumor itself, from the the body, or from a combination of both.

Methods. Breath samples were collected from 16 subjects that were diagnosed with lung cancer and 11 healthy volunteers. The breath from sick subjects was collected prior to any treatment and three weeks after tumor resection. The "healthy" population is healthy according to subjective patient's data (the person has no cancer according to his own knowledge at the moment of the breath collection). The breath of volunteers was examined by means of gas chromatography linked with mass spectrometry technique (GC-MS) as well as NaNose® - an electronic nose device that is based on molecularly-modified gold nanoparticles - developed in our research group. Pattern recognition methods, such as Principle Component Anlysis (PCA), were used then to analyze the results obtained from GC-MS and NaNose® and to correlate the results with the clinical data.

Results. GC-MS results showed a group of 30 VOCs in the breath of lung cancer patients prior to any kind of treatment. The majority of the compounds were methylated alkanes and benzenes.⁶ The NaNose® have shown excellent discrimination between the breath of lung cancer patients and that of healthy controls, with no need for preconcentration of the lung cancer biomarkers in an atmosphere of high humidity. In contrast, no discrimnaitaion was obtained between breath samples that were collected from lung cancer patinets before and 3 weeks after tunmor resection. GC-Ms results hints that a period of three weeks is not sufficienet for decreasing the VOCs in the patinets body, except in the case of isoprene and decane⁷, but longer period might do so.

Conclusions. The NaNose® technology has a high potential for assessing lung cancer via simple exhalation procedure. The results provide a launching pad towards obtaining inexpensive, compact tool that is amenable to widespread screening and that has a potential

for direct and real-time monitoring (2-3 minutes only). Still, further efforts are required to adapt this technology for follow-up purposes, especially after tumor resection. These achievements stand in consistency with the requirements of society for rapid and early diagnosis of diseases as a part of therapeutic approach and facilitating rapid treatment.

Acknowledgements. The research was funded by the Marie Curie Excellence Grant of the European Commission's FP6 program, the Alfred Mann Institute, the Israel Cancer Association, and the Technion's Russell Berrie Nanotechnology Institute. We thank Irena Dvorkind, and Orna Barash (Technion-IIT) for assistance and fruitful discussions. HH holds the Horev Chair for Leaders in Science and Technology.

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Book of Abstracts

Student Talk

In Situ Mapping of Amorphous Calcium Phosphate Transformation into Crystalline Mineral in the Fin Bones of Zebrafish: From the Cell to the Bone

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The most widespread skeletal mineralized tissue among vertebrates is represented by the bone family of materials; one of the most complex products of biological engineering. Its basic building block, the mineralized collagen fibril, is composed of spatially organized collagen protein fibrils, impregnated with aligned nanometer-size crystallites of a calcium phosphate mineral, carbonated hydroxyapatite.

The continuously elongating fin bony rays of the Tuebingen long fin zebrafish represent a spatially and temporally resolved bone growth system that largely consists of newly-formed bone. It was thus used to investigate the initial stages of skeletal bone mineralization. These encompass the characterization of the first deposited mineral and its transformation into the mature crystallites of bone within the organic framework, as well as identification of mineral delivery and deposition mechanisms. These fundamental issues involved in bone biomineralization have been highly debated for decades [2,3]. We employed high resolution electron microscopy imaging and analysis of extracted mineral particles and demonstrated the presence of an abundant amorphous calcium phosphate phase in the newly-formed fin bones. Our data suggest that the amorphous phase may be a transient precursor which transforms into the mature crystalline mineral [4]. Observations of freeze-fractured hydrated fin bones using cryo-SEM imaging reveal a growth zone, composed of aligned collagen fibrils infused by 200-500 nm globular entities. These entities are composed of mineral nano-spheres. Spatially resolved small angle X-ray scattering and diffraction measurements show the presence of a phase composed of spheres estimated as 12 nanometers in diameter, associated with a broad diffuse scatter in the wide-angle region that is present in the newly-formed bones. This signal is resolved into a clear crystalline diffraction pattern and a typical bone-particle scattering in the more mature parts of the ray. These complementary observations point to the presence of a transient disordered calcium and phosphate containing mineral phase, which we speculate is delivered in the form of spherical particles. These mineral phases subsequently become more ordered and form aligned plate-shaped crystals of carbonated hydroxyapatite, typical of mature bone.

I thank Dr. Salim Seyfried and Dr. Gil Levkowitz for providing the animals. The micro-X-ray studies were conducted at Helmholtz-Zentrum Berlin für Materialien und Energie and were supported by the European Integrated Infrastructure Initiative I3 in FP6. The electron

microscopy studies were conducted at the Irving and Cherna Moskowitz Center for Nano and Bio-Nano Imaging, Weizmann Institute of Science. I acknowledge the support by the Israeli Council for Higher Education. This research was supported by a grant from the Minerva Foundation.

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Book of Abstracts

Student Talk

NMR STUDY OF MODEL SYSTEM OF PYRIDOXAL-5'-PHOSPHATE DEPENDENT ENZYMES

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Pyridoxal-5'-phosphate (PLP) is a cofactor in many enzymes involved in amino acids transformations such as decarboxylation, racemisation and transamination among others. PLP is bound covalently through an imine bond with an ϵ -amino group of a lysine side chain residue in the active site forming an internal aldimine. We have previously studied the protonation states of PLP aldimines showing the coupled protonation of the ring nitrogen to the phenolate in the PLP moiety of the aldimine [1]. The internal aldimine is the starting point of PLP dependent enzyme's catalytic cycle. The first step consists in the transformation from the internal aldimine to the external aldimine formed between the PLP cofactor and the incoming amino acid. This is called the transaldimination. Until now, no clear mechanism has been drawn out in the literature. Snell and Jenkins [2] first postulated that transamination proceeds *via* a direct addition of the incoming amino acid to the internal aldimine forming a geminal diamine. However, other authors have proposed a required hydrolysis of the internal aldimine liberating free PLP to react with the amine group of the incoming amino acid [3]. The internal and external aldimines of PLP dependent enzymes were modeled by the aldimine stemming from the reaction in aqueous solution at pH 9 of ^{15}N enriched poly-L-lysine at the ϵ -position with PLP strategically ^{13}C enriched at the aldehyde group. ^{13}C and ^{15}N solid state NMR studies of lyophilized samples of this model system supports that the transaldimination occurs through the hydrolysis of the internal Schiff base forming PLP which is then free to react with an incoming substrate amino acid.

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Acknowledgements: Peter Tolstoy and Sharif Shasad

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