

# HYDROGEN FOR THE FUTURE

*Marie Curie Research Training Network 'Hydrogen'*  
*The 3<sup>rd</sup> RTN Meeting*

**21–25 Oct 2009**  
**Hotel Intercontinental**  
**Warsaw POLAND**

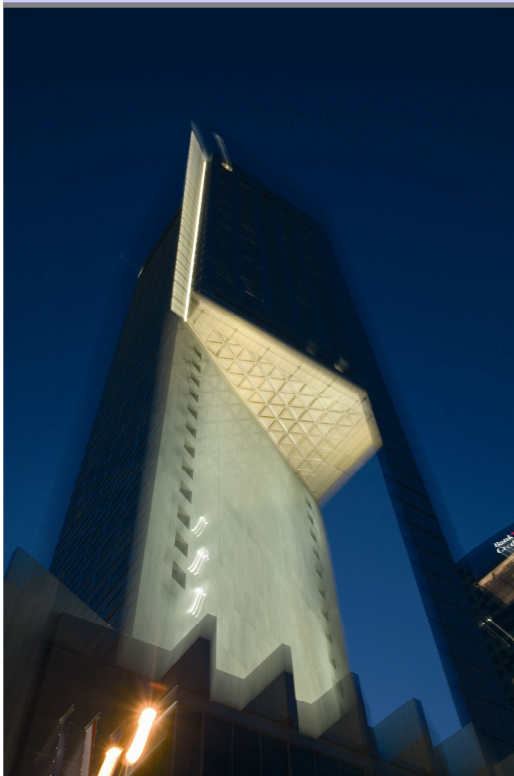


**EU 6FP: MRTN-CT-2006-032474**

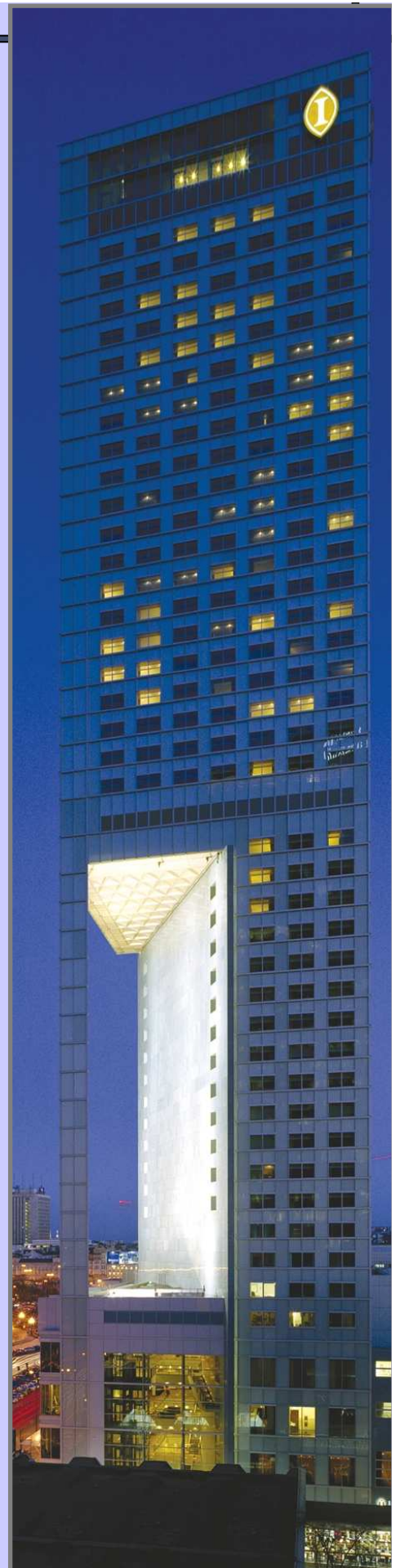
**INTERCONTINENTAL\*\*\*\***

**Emilii Plater Str. No. 49**

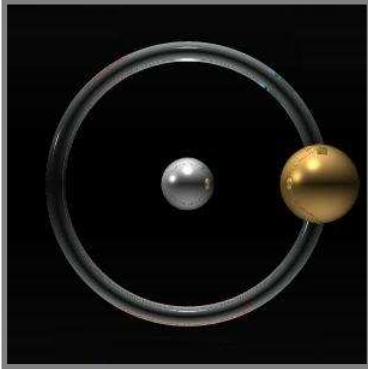
**00-125 Warsaw POLAND**



***HYDROGEN FOR THE FUTURE, The 3rd  
RTN Meeting, 21-25 Oct 2009, Warsaw Poland***



# HYDROGEN: ENERGY OF THE FUTURE



*HYDROGEN FOR THE FUTURE, The 3rd RTN Meeting, 21–25 Oct 2009, Warsaw Poland*

## MARIE CURIE RTN: 2006–2011



hydrogen a Marie Curie Research Training Network

<http://www.mcrtn-hydrogen.eu/>

I: Amsterdam NL 2007

II: Reykjavik ICE 2008

III: Warsaw PL 2009

IV: Leiden NL 2010

**$^{84}\text{Po}$  Polonium**



**Maria SKŁODOWSKA-  
CURIE (1867–1934)**

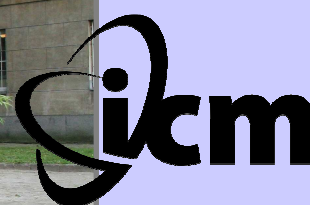
*HYDROGEN FOR THE FUTURE, The 3rd RTN Meeting, 21–25 Oct 2009, Warsaw Poland*

## The Univeristy of Warsaw



<http://www.uw.edu.pl/>

## LTNFM: ICM & Faculty of Chemistry



<http://ltnfm.icm.edu.pl/>

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**21.10 'Day 0'**

**17:30–18:30** visit to unique  
Warsaw **pH-toplasticon**,  
Aleje Jerozolimskie Str.,  
No. 51 (2 groups max. 24  
pers.)

**18:40** bus leaving from  
hotel for **Museum of Maria  
Skłodowska–Curie**, Freta  
Str., No.16

**19:00–20:00** visit at  
Museum incl. film show

**20:00**→ wandering thru  
**Old Town of Warsaw**  
There will be **NO** bus  
service back to hotel

## WARSZAWA SPRZED 100 LAT

ZE ZBIORÓW DANUTY SZLAJMER

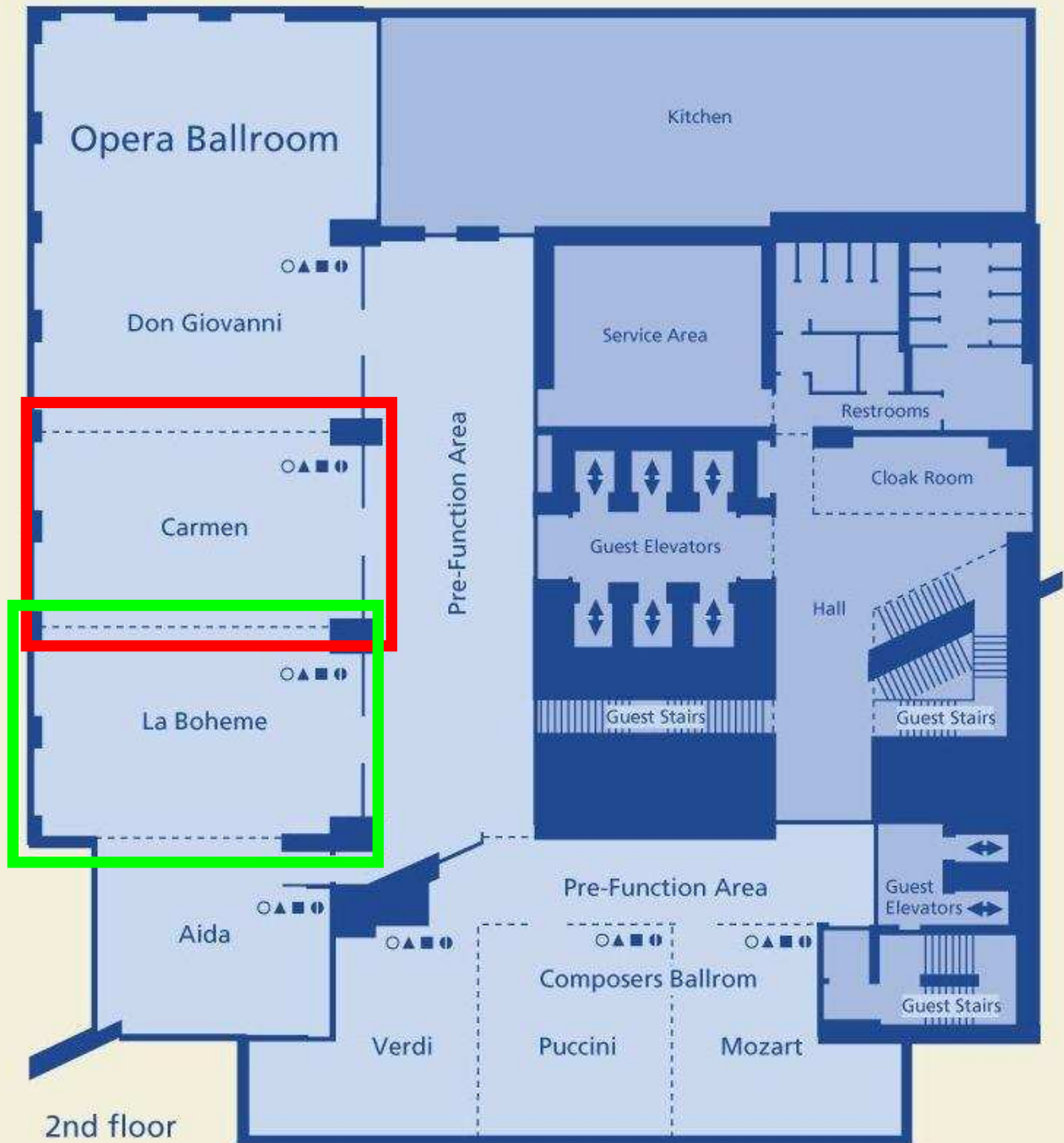


**FOTOPLASTIKON**  
WARSZAWSKI  
AL. JEROZOLIMSKIE 51 – OFICyna

24 WRZEŚNIA – 21 PAŹDZIERNIKA WSTĘP: 1 ZŁ

FOTOPLASTIKON JEST CZYNNY CODZIENNIE, OPRÓCZ WTORKÓW 10.00–18.00  
THE WARSAW STEREOCORE IS OPEN DAILY (EXCEPT TUESDAYS) 10.00 A.M.–6.00 P.M. TICKET: 1 PLN

## Lecture Halls



**CARMEN:** Oct 22 **LA BOHEME:** Oct 23, 24, 25

## 22.10 'Day 1', room CARMEN (2<sup>nd</sup> floor)

9:15-9:25 Welcome – Marek Niezgódka

9:25-9:55 Wojciech Grochala „Welcome to Poland, welcome to Warsaw!”

9:55-10:00 Organizers' “Reminders for the day”

10:00-11:00 SESSION 1 **Chair: Adriana Paracchino**

Florian Le Formal (EPFL) *Solar Driven Water Splitting : Principle and An Example with Hematite.*

Jeremie Brillet (EPFL) *Innovative nanostructured photoanodes for Solar energy conversion.*

11:00-11:20 morning coffee break

11:20-12:20 SESSION 2: **Chair: Nicola Naujoks**

Adriana Paracchino (EPFL, guest speaker) *Exploration of a new class of p-type oxides for hydrogen evolution in photoelectrochemical water splitting.*

Rafael Martins (CHA) *Nanostructuring Photoanodes for Hydrogen Production via Water Splitting.*

12:30-13:30 lunch: restaurant *Downtown*, 1<sup>st</sup> floor

13:30-14:30 SESSION 3: **Chair: Geert-Jan Kroes**

Peter J. Kluepfel (UI) *Self-interaction corrected energy functionals -- An interpolating between two regimes of electronic structure.*

Alvaro Valdes de Luxan (LEI) *Cluster study of the Photo-Oxidation of Water on TiO<sub>2</sub> Surface.*

14:30-14:50 afternoon coffee break

14:50-15:50 SESSION 4: **Chair: Ilaria Pino**

Isabela Man (DTU) *Competitive chlorine and oxygen evolution at rutile(110) surfaces (DFT).*

Ivan Ljubic (OX) *Towards Understanding Mechanism of Reversible Hydrogen Storage in Transition Metal Doped Sodium Alanate.*

15:50-16:00 **prize for the best ESR & ER speech of the day**

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**17:30** leaving from hotel to the **Palace of Culture and Science** (sunset view of Warsaw from its very roof, groups of 8 persons)

**19:00**–22:00 Informal meeting **Hard Rock Cafe**, Złota Str., No. 59 ('open bar')



## 23.10 'Day 2', room LA BOHEME (2<sup>nd</sup> floor)

8:30-9:50 **PI Meeting**

9:55-10:00 Organizers' "Reminders for the day"

10:00-11:00 SESSION 1. **Chair: [Ewa Banach](#)**

Flavio Pendolino (EMPA) *The "Boron effect" in the decomposition of light metal borohydride.*

Tomasz Jaroń (WAR, guest speaker) *Storage of hydrogen in lightweight  $Y(BH_4)_3$ .*

11:00-11:20 morning coffee break

11:20-12:20 SESSION 2. **Chair: [Andrew J. Churchard](#)**

Radostina V. Genova (WAR) *Probing hydrogen storage properties of materials based on yttrium and ytterbium.*

Ewa Banach (SHL) *Synthesis and characterization of Al/ZIF-8 composites.*

12:30-13:30 lunch: restaurant *Downtown*, 1<sup>st</sup> floor

13:30-14:30 SESSION 3. **Chair: [Alvaro Valdes de Luxan](#)**

Jian-cheng Chen (LEI)  *$H_2$  dissociation and formation of  $AlH_3$  on  $c(2 \times 2)$ -Ti/Al(100) surfaces.*

Andrew J. Churchard (WAR) *Molecular catalysts for thermal decomposition of complex hydrides.*

14:30-14:50 afternoon coffee break

14:50-15:50 SESSION 4. **Chair: [Isabela Man](#)**

Nicola Naujoks (CHA) *Investigating hydrogen storage in thin films and nanoparticles.*

Loránd Románszki (CHA) *3-D porous templates to study hydrogen storage in nanoparticles by QCM.*

15:50-16:00 **prize for the best ESR & ER speech of the day**

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**17:30** bus leaving from hotel to [Oycowizna restaurant](#), Słoneczna Str., No. 241, 05-506 Lesznowola/ Magdalenka (ca. 15 km from hotel)

19:00–23:00 **conference banquet**

**23:00** bus leaving back to hotel

## 24.10 'Day 3', room LA BOHEME (2<sup>nd</sup> floor)

9:55-10:00 Organizers' "Reminders for the day"

10:00-11:00 SESSION 1. Chair: [Michael Zach](#)

Lucjan Piela (WAR) *H<sub>2</sub> molecule in detail.*

Dinko Chakarov (CHA) *It happens on the surface.*

11:00-11:20 morning coffee break

11:20-12:20 SESSION 2. Chair: [Marten Bjorketun](#)

Igor Zoric (CHA) *Thermodynamics and kinetics of hydriding and dehydriding of metallic nanoparticles: Does the size matter?*

Ronald Griessen (VU, Netherlands) *Tuning thermodynamics of M-H (nano)systems with elastic constraints.*

12:30-13:30 lunch: restaurant *Downtown*, 1<sup>st</sup> floor

13:30-14:30 SESSION 3. Chair: [Peter P. Edwards](#)

Armand Budzianowski (WAR) *Tiny crystals and giant pressure: David and Goliath in the lab.*

Dominik Kurzydłowski (WAR) *New Polymorphs of Silane, SiH<sub>4</sub> Accessed by High Pressure: A Computational Study.*

14:30-14:50 afternoon coffee break

14:50-15:50 SESSION 4. Chair: [John A. Turner](#)

Hans Geerlings (SHL) *A short introduction to CO<sub>2</sub> capture and sequestration.*

Peter P. Edwards (OX, UK) *Can we make a materials difference to a sustainable energy future?*

15:50-16:00 prize for the best training speech of the day

Poster mini-session during whole day:

Przemysław Malinowski (WAR); Karol Fijałkowski (WAR).

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16:15 bus leaving from hotel for [Museum of Warsaw Uprising](#)

16:30–19:00 visit at Museum (2 groups, ENG guides)

19:15 bus leaving back to hotel

## 25.10 'Day 4', room LA BOHEME (2<sup>nd</sup> floor)

**9:55-10:00** Organizers' "Reminders for the day"

**10:00-11:00** SESSION 1. Chair: [Arndt Remhof](#)

Łukasz Dobrzycki (WAR) *Headache of hydrogen position determination by diffraction techniques.*

Mariana Derzsi (WAR) *Lighter balls kicking heavier ones: what can we learn from neutron's impact on H-rich materials?*

**11:00-11:20** morning coffee break

**11:20-12:20** SESSION 2. Chair: [Hannes Jonnson](#)

Sebastien Rives (LEI) *MD simulation of hydrogen storage in sII clathrates hydrates: Effect of promoter molecules and diffusion of H<sub>2</sub>.*

John A. Turner (NREL, USA) *Hydrogen Production from Photoelectrochemical Cells: Theoretical considerations and experimental results.*

**12:30-13:30** lunch: restaurant *Downtown*, 1<sup>st</sup> floor

**13:30-14:30** SESSION 3. Chair: [Mariana Derzsi](#)

Hannes Jonnson (UI) *The rate of thermally activated transitions, such as diffusion and chemical reactions.*

Marten Bjorketun (DTU) *Hydrogen evolution: a first-principles perspective.*

**14:30-14:50** afternoon coffee break

**14:50-15:50** SESSION 4. Chair: [Armand Budzianowski](#)

Arndt Remhof (SFLMTR) *Hydrogen dynamics in light borohydrides.*

Stanisław M. Filipek (IChF PAN, WAR) *Unusual behavior of the most simple element; hydrogen-metal systems under high pressures.*

**15:50-16:00** prize for the best training speech of the day

**16:00-16:15** closing remarks & farewell

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**17:00-** leaving (cars, taxi) for [gokart contest](#) in Bemowo Mall (18:00-20:00, private fun, optional) <http://www.pole-position.pl/>