

UNIVERSITÀ DELLA CALABRIA



# XXV Congresso Nazionale della Società Chimica Italiana

Arcavacata di Rende  
07-12 Settembre 2014

**PROGRAMMA SCIENTIFICO  
PERCORSO ENERCHEM**

Percorso **EnerChem** al XXV Congresso della Società Chimica Italiana  
Rende 7-12 settembre 2014

**Lunedì 8 settembre**

**Divisione di Chimica Fisica** (chairperson: E. Sellì, A. Sinicropi)

*Aula Caldora*

09:10 – 09:40	<b>CHF-K1:</b> Nicola Armaroli <i>From hydrocarbons to solar energy: unfolding trends for chemistry</i>
09:40 – 10:00	<b>CHF-O1:</b> Gian Luca Chiarello, E. Sellì <i>Photocatalytic Hydrogen Production</i>
10:00 – 10:20	<b>CHF-O2:</b> Roberto Comparelli, F. Petronella, A. Truppi, E. Binetti, A. Panniello, M. Striccoli, A. Agostiano, M. L. Curri <i>Colloidal nanocrystals for energy conversion applications</i>
10:20 – 10:40	<b>CHF-O3:</b> Jenny G. Vitillo, J. Ethiraj, F. Giordanino, V. Crocellà, G. Ricciardi, E. Groppo, M. Baricco, F. Bonino, S. Chavan, S. Bordiga <i>Carbon dioxide capture and recycling in microporous materials</i>
10:45 – 11:05	Coffee Break
11:05 – 11:25	<b>CHF-O4:</b> D. Costenaro, Chiara Bisio, G. Gatti, T. B. Meyer, M. Graetzel, L. Marchese <i>Porous and layered solids for the development of innovative quasi-solid electrolytes for dsc applications</i>
11:25 – 11:45	<b>CHF-O5:</b> Simona Binetti, A. Le Donne, P. Garattini, S. Tombolato, R. Mereu, M. Meschia, M. Acciari <i>Chalcogenide thin film solar cells on flexible substrates</i>
11:45 – 12:05	<b>CHF-O6:</b> Giuseppe Calogero, I. Citro, A. Bartolotta, G. Di Marco, A. Sinopoli, S. Caramori, C.A. Bignozzi, V. Petrov, A. M. Diniz, A. J. Parola, F. Pina <i>A complete study on synthetic analogues of anthocyanins as bio-inspired sensitizers for dye-sensitized solar cells</i>
12:05 – 12:25	<b>CHF-O7:</b> Sante Cospito, A. Beneduci, M. La Deda, G. Chidichimo <i>Gel polimerici elettrofluorocromici</i>

**Divisione di Chimica Teorica e Computazionale** (chairperson: G. Pacchioni)

*Aula CF2 (Cubo 32 C Ponte Carrabile)*

15:00 – 15:30	<b>TEO-K2:</b> Fabrizia Negri <i>Interplay of electronic, optical and transport properties in extended core ORGanic semiconductors: rationale from modeling</i>
15:30 – 15:50	<b>TEO-O6:</b> Sandro Jurinovich, L. Viani, S. Caprasecca, B. Mennucci <i>Energy Transfer in Light Harvesting Systems: a QM/MM-Pol Approach</i>
15:50 – 16:10	<b>TEO-O7:</b> Sofia Canola, F. Negri <i>Anisotropy of n-type charge mobility and thermal effects in crystals of a fluoro-alkylated naphthalene diimide: a computational investigation</i>
16:10 – 16:30	<b>TEO-O8:</b> Remedios Cortese, F. Ferrante, D. Duca <i>Hydrogen activation on N-doped carbon networks</i>
16:30 – 16:50	Coffee Break
16:50 – 17:10	<b>TEO-O9:</b> Elisa Albanese, B. Civalleri, M. Baricco <i>Tuning the Stability of Ca(BH<sub>4</sub>)<sub>2</sub> by the Inclusion of Additives: A Computational Study</i>
17:10 – 17:30	<b>TEO-O10:</b> Roberto Schimmenti, R. Cortese, D. Duca <i>A computational approach to study Aqueous Phase Reforming</i>
17:30 – 17:50	<b>TEO-O11:</b> Lorenzo Canti, A. Fraccarollo, G. Gatti, M. Errahali, M. Cossi, L. Marchese <i>Monte Carlo Modeling of Carbon Dioxide Adsorption in Porous Aromatic Frameworks</i>

**Martedì 9 settembre**

**Divisione di Elettrochimica** (chairperson: V. Baglio, P. Mustarelli)

*Aula Chimica (Cubo 17C Ponte Carrabile)*

15:00 – 15:20	<b>ELE-O16:</b> Eliana Quartarone, S. Angioni, D. C. Villa, P. Mustarelli, A. Magistris <i>Polybenzimidazole-based membranes for HT-PEMFCs</i>
15:20 – 15:40	<b>ELE-O17:</b> Isabella Nicotera, K. Angieli, C. Simari, V. Kosma, L. Coppola, V. Baglio <i>Layered nanostructures for composites hybrid membranes in fuel cell application: investigation of water and methanol transport properties</i>
15:40 – 16:00	<b>ELE-O18:</b> Valentina Perazzolo, C. Durante, R. Pilot, Z. Jian, R. Bozio, G. Granozzi, A. Gennaro <i>Nitrogen-doped mesoporous carbons: activity towards oxygen reduction</i>
16:00 – 16:20	<b>ELE-O19:</b> Michael Ongaro, J. Roche, A. Kuhn, P. Ugo <i>Dissymmetric modification of micro- and nanoparticles for energy conversion</i>
16:30 – 16:50	Coffee break
16:50 – 17:10	<b>ELE-O20:</b> Italo Doberdò, A. Maheshwari, M. Santarelli, S. Bodoardo, N. Penazzi <i>Mathematical modeling and simulation of Li-ion battery</i>

## **Mercoledì 10 settembre**

### **Divisione di Chimica Industriale**

*University Club*

09:00 – 09:40	<b>IND-K4:</b> Roberto Fusco, D. Testa <i>ENI research on next generation photovoltaics</i>
09:40 – 10:00	<b>IND-O20:</b> Federico Bella, R. Bongiovanni <i>Photopolymers for Grätzel's solar cells</i>
10:00 – 10:20	<b>IND-O21:</b> Giuseppe Barbieri, E. Drioli, A. Brunetti <i>Membrane reactors for innovating hydrogen stream upgrade</i>
10:20 – 10:40	<b>IND-O22:</b> Francesco Basile, D. Barbera, P. Benito, G. Fornasari, R. Mafessanti, M. Monti, A. Vaccari <i>New structured catalysts and system for H<sub>2</sub> and syngas production</i>
10:45 – 11:05	Coffee Break
<i>Chairperson</i>	
11:05 – 11:25	<b>IND-O23:</b> Alessandro Donazzi, D. Pagani, A. Lucotti, M. Tommasini, A. Beretta, G. Groppi, C. Castiglioni, P. Forzatti <i>Kinetic and Raman study in the CPO of C<sub>3</sub>H<sub>8</sub>, C<sub>3</sub>H<sub>6</sub> and n-C<sub>4</sub>H<sub>10</sub></i>
11:25 – 11:45	<b>IND-O24:</b> Gianni Golemme, A. Santaniello <i>Mixed Matrix Membranes for Gas Separation</i>

## **Giovedì 11 settembre**

### **Divisione di Chimica Inorganica** (chairperson: M. Peruzzini)

*Aula E1 (Cubo 5 B Ponte Carrabile)*

15:00 – 15:30	<b>INO-K10:</b> Francesco Vizza, M. Bellini, M. Bevilacqua, M. Innocenti, A. Lavacchi, A. Marchionni, H. Miller, J. Filippi, L. Wang <i>Energy &amp; Chemicals from Renewable Resources by Electrocatalysis</i>
15:30 – 15:50	<b>INO-O36:</b> Gaetano Granozzi <i>DECORE: a new european project aiming at innovative DEFCs operating at intermediate temperatures</i>
15:50 – 16:10	<b>INO-O37:</b> Carlo Nervi, F. Franco, C. Cometto, L. Nencini, C. Sun, R. Gobetto <i>Exploring ORGanometallic catalysts for photo- and electro-reduction of CO<sub>2</sub></i>
16:10 – 16:30	<b>INO-O38:</b> Elena Rebollo, C. Mortalò, S. Boldrini, S. Barison, M. Fabrizio <i>BaCe<sub>1-x</sub>Zr<sub>x</sub>Y<sub>0.15</sub>O<sub>3-δ</sub> – Y/Gd -Doped CeO<sub>2</sub> cer-cer composites for H<sub>2</sub> separation</i>
16:30 – 16:50	<b>INO-O39:</b> Nicola Dalle Carbonare, S. Caramori, C. A. Bignozzi <i>Hematite photoanodes modified with a Fe(III) water oxidation catalyst</i>
16:50 – 17:10	<b>INO-O40:</b> I. Corbucci, A. Petronilho, H. Müller-Bunz, L. Rocchigiani, M. Albrecht, <b>Alceo Macchioni</b> <i>Dramatic effect of Me to Oct substitution in the activity of pyridine-carbene iridium water oxidation catalysts</i>

## **Venerdì 12 settembre**

### **Divisione di Chimica Organica** (chairperson: M. Maggini)

*Aula Magna “Beniamino Andreatta” del Centro Congressi*

11:15 – 11:30	<b>ORG-O54:</b> Norberto Manfredi, B. Cecconi, C. Coluccini, F. Melchiorre, G. Giannotta, P. Biagini, A. Abbato <i>Multibranched organic sensitizers for photovoltaics and solar fuels</i>
11:30 – 11:45	<b>ORG-O55:</b> Tiziana Del Giacco, S. Basilic, F. Elisei, R. Germani <i>Acridinium-based sensor as fluorescent photoinduced electron transfer probe for proton detection modulated by anionic micelles</i>
11:45 – 12:00	<b>ORG-O56:</b> Davide Bonifazi <i>Engineering organic materials through serendipity</i>