Università degli Studi di Torino
Dipartimento di Chimica

chimica | Commissione Ricerca

DAYS

Chemistry for Energy

martedì 10 giugno aula D1, ore 9:15 aula D1

9.00-9.15 **Introduction to Energy Center**
Marcello Baricco

9:15-9:30 Carbon dioxide capture and recycling in microporous materials
Silvia Bordiga (10 min di discussione)

9:40-9:55 In silico" Materials design for energy: mith or reality?
Gabriele Ricchiardi (10 min di discussione).

10:05-10:20 Nuove idee e nuovi materiali per il light harvesting in sistemi fotocatalitici potenzialmente attivi nelle reazioni di fotosintesi artificiale.
Elio Giamello (10 min discussione)

10:30-10:40 Commissione Spokes

10:40-11:10 Coffee break (discussion)

11:10-11:25 Strategie per il controllo della decomposizione di boroidruri metallici: studio computazionale ab-initio.
Bartolomeo Civalleri (10 min discussione)

11:35-11:50 Metallic materials for energy storage, saving and harvesting
Alberto Castellero (10 min discussione)

12:00-12:15 Dibranched Squaraines as NIR-sensitizers for DSC.
Guido Viscardi (10 min discussione)

12.30 **End of the day**

Carbon dioxide capture and recycling in microporous materials

Silvia Bordiga, Francesca Bonino, Jenny G. Vitillo; PhDs and Post-docs

Carbon dioxide is generally recognized as the most important greenhouse gas. Its monotonic increasing trend is at the basis of the increasing research interest in materials that capture CO_2, either by physical ad-sorption or by dissociative chemi-sorption. Nevertheless, being the annual amount of CO_2 released of the order of gigatons, to find an effective way to reuse it as valuable chemical reagent is a key point in the global warming research. However, the low oxidation state of carbon strongly hinders CO_2 reactivity. In the present work, different original strategies aimed to increase the performances of materials used in all the steps of carbon dioxide recycling life are presented. In particular, the possibility to increase affinity of microporous materials for storage and separation toward CO_2 was explored by introduction of chemical functionalities as polarizing centres (cations with coordination vacancies or amines) and by metal oxide coating. Moreover, recent results of CO_2 reduction (in a microporous phase of γ-$Mg(BH_4)_2$) and CO_2 reactivity with ethyleneoxide (in a poly-aionic liquid) will be described.

Computational materials and process design for energy and the environment: mith or reality

Gabriele Ricchiardi, Oliver Inderwildi

The ability of computational methods to deliver reliable accurate properties for molecular and cristalline systems of increasing complexity is evident. It is nowadays often easier and less expensive to calculate an observable as it is to actually measure it.
Molecular modelling i soften associated to the concept of „design“ (as in engineering design): materials design, process design, drug design…
We often motivate our own work in catalysis, hydrogen storage or CO2 capture , as part of a design effort with the objective of creating better energy technologies.
However the gap between molecular scale simulations and practical applications remains a large one. This short contribution reviews some cases in which this gap has been bridged and molecular simulations can be used to take practical decisions in the field of energy and the environment.

Nuove idee e nuovi materiali per il light harvesting in sistemi fotocatalitici potenzialmente attivi nelle reazioni di fotosintesi artificiale.

Elio Giamello, Maria Cristina Paganini, Stefano Livraghi, Mario Chiesa.

Questo contributo intendere mettere a fuoco alcune problematiche relative ai sistemi di harvesting della luce solare in sistemi di interesse foto catalitico. L’approccio da noi seguito punta su ossidi semiconduttori od isolanti di alta stabilità chimica e si basa sul “band gap engineering”degli ossidi stessi attraverso modificazione chimica della matrice. Saranno presentati alcuni esempi di valenza metodologica riguardanti sia la riduzione del gap di un ossido che la creazione di stati intermedi in band gap.

Strategie per il controllo della decomposizione di boroidruri metallici: studio computazionale ab-initio

Bartolomeo Civalleri, Piero Ugliengo, Marcello Baricco, Marta Corno, Elisa Albanese

Negli ultimi anni è cresciuto l'interesse verso i boroidruri metallici come possibili materiali per l'immagazzinamento di idrogeno. Nonostante l'alto contenuto in peso di idrogeno, soprattutto per i boroidruri con metalli leggeri (es. Li, Na, Mg,...), alcuni di essi sono troppo stabili per poter essere usati in applicazioni reali. Inoltre, la cinetica di decomposizione non è sempre favorevole e i cammini reattivi possono portare a prodotti che riducono la reversibilità del processo di decomposizione. All'interno di alcuni progetti europei, è stato quindi intrapreso uno studio computazionale ab-initio di questi materiali con l'obiettivo di capire come favorirne la termodinamica di decomposizione. A questo scopo, sono state studiate diverse strategie per il controllo dell'entalpia di decomposizione di boroidruri di metalli alcalini (Li, Na) e alcalino-terrosi (Mg, Ca). In particolare: la sostituzione anionica e cationica, nano-strutturazione e nano-confinamento, e l'aggiunta di additivi, come metalli di transizione (Ni, Cu, ...). In questo contributo verranno discussi i principali risultati ottenuti e le attività in corso, evidenziando le capacità predittive della modellizzazione.

Metallic materials for energy storage, saving and harvesting

M.Baricco, L.Battezzati, A.Castellero, G.L.Fiore, P.Rizzi, Postdocs and PhD students

Environmental and geo-politic issues push towards both energy sources/carriers alternative to traditional fossil fuels, and higher efficiency in energy management. In this context, suitable metallic materials can give a contribution in the fields of 1) energy storage, 2) energy saving and 3) waste heat recovery.

1) Metallic materials have potential applications in hydrogen storage because of their high volumetric density, low cost and affordable processing routes. In view of real applications, the reaction kinetics of hydrogen absorption and desorption in metals and alloys need to be optimized with suitable additives in order to operate at moderate pressure and temperature.

2) Fe- and Co- based metallic glasses show low values of coercivity because of their amorphous structure. Thus, they can substitute conventional soft magnets in transformers reducing magnetic losses upon service.

3) Waste heat can be recovered exploiting the thermoelectric effect in semiconducting metallic compounds which allows the conversion of a thermal gradient into electrical energy. The development of a cheap, efficient and environmentally friendly technology based on thermoelectricity is an open issue that requires a multidisciplinary approach.

For each topic we will present the research lines, a selection of results, the current and potential collaborations.

Dibranched Squaraines as NIR-sensitizers for DSC.

Nadia Barbero, Claudia Barolo, Pierluigi Quagliotto, Guido Viscardi

The strong request for renewable energy sources has recently boosted the interest in photovoltaic devices. Among all the organic and hybrid organic-inorganic solar cells, Dye-sensitized Solar Cells (DSCs) have demonstrated one of the highest conversion efficiencies and a mature research and development plan. DSCs have several advantages: improved performances at low light intensities and diffuse light, color tunability, and transparency; therefore, they are very appealing for building-integrated photovoltaics (BIPV).

Metal-free organic sensitizers are accessible by simple synthetic approaches and well established purification procedures. Structurally, they can be simply modified and functionalised in order to obtain the desired spectroscopic properties between 400–700 nm.

In this talk we present the synthesis and the optical and photovoltaic characterization of a series of symmetric dibranched squaraine-based sensitizers as a low cost and photostable alternative to the classical unsymmetrical NIR dyes. A panchromatic light harvesting was also obtained by an accurate tuning of the employed molecular moieties on the squaraine framework (Figure 1). The effect of the length of the alkyl chains as well as the effect of the functional groups on the anchoring mode and TiO_2 interaction will be also discussed.

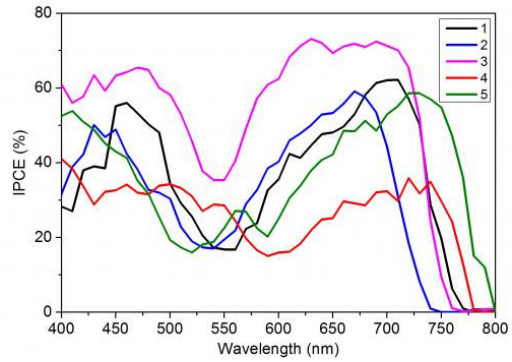

Figure 1: IPCE spectra of selected panchromatic squaraine dyes.