Energy Harvesting & Storage
Room Naupaka Salon 6-7 - Session EH-MoE

Process
Moderator: Paul Dastoor, University of Newcastle, Australia

5:40pm **EH-MoE1 Surface Engineered Smart Optical Nanostructures for Energy Saving and Thermal Control**, *Ludvik Martinu,* Montreal Ecole Polytechnique, Canada **INVITED**

Optical coating (OC) applications represent a multibillion dollar market worldwide; they range from antireflective (AR) coatings found in most optical components and low emissivity windows in buildings and automobiles to narrowband optical interference filters used in telecommunications. As the range of applications of OCs continuously broadens and extremely attractive market opportunities arise, it is becoming increasingly important to develop new nanostructured thin film materials with specific multifunctional properties. Further progress in this fast evolving field is strongly stimulated by a simultaneous action of two forces: a) the "pulling force" represented by the economic, technological and societal needs, including sustainable development, and b) the "pushing force" related to the curiosity-driven nanotechnology combining new design concepts of materials and devices, fabrication processes and innovative characterization tools, where the only limitation frequently appears to be our imagination.

This presentation will describe a holistic approach to OCs based on a broad and in depth knowledge of the interplay between the design, material, process and performance with respect to specific applications and coating system durability. It will review the progress and future opportunities for the use of nanostructurally-controlled architectures, advanced deposition techniques including high power impulse magnetron sputtering (HiPIMS), atomic layer deposition (ALD), glancing angle deposition (GLAD) and tailored plasma- and ion-surface interactions, as well as complex systems implementing active (smart, tunable thermochromic and electrochromic) materials.

These trends will be illustrated by examples from the field of advanced glazings for energy saving using smart windows, and smart radiators with self-tuned emissivity for the thermal management in satellites

6:20pm **EH-MoE3 Carbon Capture by Metal Oxides: Unleashing the Potential of the (111) Facet**, *Ryan Richards,* Colorado School of Mines, USA*; S. Shulda,* National Renewable Energy Laboratory, USA*; G.A. Mutch,* Newcastle University*; J.A. Anderson, D. Vega-Maza,* University of Aberdeen

Carbon capture, utilisation and storage is a portfolio of processes to combat climate change. The capacity of sorbents proposed for low temperature carbon capture is entirely limited to surface interaction, resulting in a race to produce ever increasing surface areas - exemplified by metal-organic frameworks.

Metal oxides have a diverse range of electronic and physical properties that make them useful for a variety of applications such as semiconductors in diodes, electro- and thermo-chromics, catalysis and Li ion batteries --to name a few. One of the simplest structures of metal oxides is the rock-salt structure that are face-centered cubic crystals with the metal ion surrounded by six nearest-neighbor oxygen ions and vice versa. Amongst the rock-salt metal oxides, MgO is the most widely studied and is the second most abundant compound in the Earth's crust at 35% (behind silica which is 42%). [1] Due to surface area reduction by sintering, solid metal oxides generally exhibit reduced adsorption capacity for carbon capture following high temperature exposure.

The preponderance of literature studies involving the properties of metal oxides has been conducted on the (100) surface because this surface is the most readily obtained and most thermodynamically stable form for most rock-salt metal oxides. The (100) surface is a checkerboard of alternating metal cations and oxygen anions. While most methods produce materials dominated by (100) surfaces, decomposition of metal hydroxides such as $Mg(OH)_2$ can initially yield materials with hydroxylated (111) surfaces via topotactic dehydration. [1-3] Following the development of techniques that allow for the deliberate preparation of materials with primarily (110) and (111) surfaces, came interest in potentially new properties of these surfaces. [4,5]

The (111) facet of MgO however, exhibits a high concentration of low coordinate sites. [4,5] In recent work, MgO(111) nanosheets displayed high capacity for CO_2, as well as a ≈ 65% increase in capacity despite a ≈ 30% reduction in surface area following sintering (0.77 mmol g^{-1}@ 227 m^{2}g^{-1}vs 1.28 mmol g^{-1}@ 154 m^{2}g^{-1}). [6] These results, unique to MgO(111) suggest

intrinsic differences in the effects of sintering on basic site retention. Spectroscopic and computational investigations provided a new structure-activity insight; the importance of high temperature activation to unleash the capacity of the polar (111) facet of MgO. In summary, we present the first example of a faceted sorbent for carbon capture and challenge the assumption that sintering is necessarily a negative process; here we leverage high temperature conditions for facet-dependent surface activation.

6:40pm **EH-MoE4 Graphene Oxide-cellulose Nanocrystal Sponge as a Tunable Platform for Contaminant and Pathogen Removal from Water**, *Nathalie Tufenkji, N. Yousefi, R. Allgayer, A. Filina,* McGill University, Canada

Graphene oxide (GO) sponges are a new class of sorbents for removal of a diverse range of contaminants from water. The immobilization of GO in a solid porous macrostructure eliminates the requirement for removal of the otherwise stable colloidal GO from the treated water. Unlike colloidal GO, solid macrostructures can be easily stored, transported and manipulated. Although much progress has been made on forming high surface area and multifunctional GO sponges, synthesizing mechanically robust multifunctional sponges, especially in wet state, is a challenge. We report the preparation of an ultrastrong GO-based sponge strengthened with cellulose nanocrystal (CNCs) – natural nanorods isolated from wood pulp – using a green synthesis method with the aid of excess vitamin C (VC). VC acts as a natural reducing agent, whereas CNCs provide a scaffold that links the reduced GO (rGO) nanosheets together, resulting in an exceptionally stiff nanocomposite. During sponge synthesis, undissolved excess VC grains act as soft templates, yielding nanocomposites with hierarchical pore architecture, even in the core of large sponges as confirmed by micro and nano X-ray tomography. The use of ultra-large GO nanosheets, as well as the interconnected hierarchical pore structure translate into sponges with a high specific surface area and large removal capacity for a wide range of contaminants such as dyes, heavy metals, and pharmaceuticals. The GO-CNC sponges exhibit excellent contaminant removal from single and multicomponent waters, in batch and continuous removal modes. Additionally, we show that the sponges of this study can be readily functionalized with antimicrobial peptides and biopolymers to enhance removal and inactivation of bacteria from contaminated water supplies.

7:00pm **EH-MoE5 Surface Science Approach For Alumina Supported Hydrodesulphurisation Catalysts**, *Anne-Félicie Lamic-Humblot,* Sorbonne Université, France*; C. Bara,* Solvay*; R. Garcia de Castro,* Sorbonne Université, France*; E. Devers, G. Pirngruber, M. Digne,* IFPEN*; X. Carrier,* Sorbonne Université, France

Since 2009, the sulphur content need to be reduced to 10 ppm in gasoline. In order to achieve this goal, hydrodesulphurisation process is efficient for now, using sulfided molybdenum (doped or not by cobalt) deposited on alumina.

In order to optimize this process, a molecular-scale understanding of the adsorption of the active phase (metal ions) is of fundamental importance. However, this objective is difficult because of the high surface area developed by the support (g-alumina) and the large number of exposed sites. One way to simplify the system is to use oriented single crystals of alumina presenting a lower number of sorption sites and well defined surface sites. As single crystals of g-alumina do not exist, we use some of a-alumina commercial wafers in order to mimic the g-alumina exposed surfaces.

Ammonium heptamolybdate complexes were deposited on the surface using conventional aqueous routes ("equilibrium" adsorption and impregnation). The samples were then calcined and sulphided. The samples were characterised (XPS, AFM) after each thermal treatment.

The sulphurisation degree was determined with sulphurisation temperature, and a correlation between the exposed sites and molybdenum sulphide is discussed. GI-EXAFS allowed us to show that the exposed surface induce in some case a certain orientation of MoS_2slabs on the surface.

Hence it is possible to conclude that the control of the industrial support morphology constitutes a way to tune the genesis of the hydrotreating catalysts sulfide phase.

7:40pm **EH-MoE7 Direct 3D Printing of Reactive Agitating Impellers for the Convenient Treatment of Various Pollutants in Water**, *Xueyan Sun,* Dalian University of Technology, China

Mass transfer plays a key role in the diffusion-controlled heterogeneous reactions. Varied efforts have been made to design the structure of

catalysts and reactors to optimize the diffusion process. Herein, a facile strategy is reported to construct highly reactive agitating impeller (denoted as AI) by employing 3D printing and a facile surface activation treatment. On the one hand, experimental results and numerical simulation analysis reveal that the 3D printing AI with appropriate structure can not only effectively eliminate external diffusion but also conveniently be separated from heterogeneous reaction systems. On the other hand, surface activation helps to significantly promote the chemical reactivity of AI for Fenton and galvanic replacement reaction, which are used to treat organic and inorganic pollutants in water, respectively. Benefiting from these cooperative merits, the integrated catalytic AI delivers a catalytic performance toward Fenton reactions as high as a homogeneous catalyst, and the removal rate for heavy metal ions is nearly 100% through galvanic replacement. This 3D printing with surface engineering strategy should also be extended to other applications, and provide new field for preparing efficient and durable heterogeneous catalysts in a more economical way.

8:00pm **EH-MoE8 BN Films for Hydrogen Permeation Barrier**, *Motonori Tamura,* The University of Electro-Communications (UEC-Tokyo), Tokyo, Japan

Cubic boron nitride (c-BN) has attracted much attention because of its outstanding physical and electrical properties. However, there are limited research data on hydrogen permeation of BN thin films that can be applied to

components of hydrogen fuel cells. Several techniques such as sputtering, laser ablation, ion-beam deposition, and plasma-enhanced chemical vapor deposition are used to synthesize c-BN films. To realize a stable c-BN structure and film stoichiometry, precise control of the plasma parameters is necessary. In this study, a magnetically enhanced plasma-ion-plating system was successfully designed and applied to produce stable c-BN films.

Hydrogen-permeation tests of BN-, SiC-, and TiN-coated Type 316L stainless steels were performed. A diffusion-limited permeation regime was confirmed on the coated samples at 573-773 K. The permeability depended on the test temperature, where high values of permeability data were obtained at high temperature. The hydrogen permeability data of SUS316L stainless steel in the temperature range of 573-773 K correlated well with results of a previous study. Our results indicate that the 1.5-micrometers-thick films of SiC, TiN, and BN were all effective in reducing the hydrogen permeability. In comparison with TiN and SiC coatings, the c-BN (cubic boron nitride) coating was most effective to reduce the rate of hydrogen permeation through stainless steel.

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