Crystal Science Seminar

Some recent structural aspects of molybdenum nitride Mo_5N_6

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Transition metal nitrides (TMN) have demonstrated their potential in heterogeneous catalysis in reactions traditionally catalyzed by noble metals [1]. They are often considered as platinoids for their close electronic properties. TMN contribute to the renewed interest in finding alternatives to these very expensive and rare noble metals (Pt, …) listed as critical raw materials.

This work aims at developing innovative syntheses to prepare nanostructured TMN from metallic clusters [2]. The use of a nanoscale precursor such as $(TBA)_2Mo_6Br_{14}$ (TBA= tetrabutylammonium) enables to reach different molybdenum nitride compositions (Mo_2N, Mo_5N_6) by thermal reaction under ammonia at relatively low temperatures. Such a novel synthetic approach highlights the prime importance of the starting material stabilizing specific stoichiometries [3-4] in comparison with the MoS_2 route. This presentation will focus on the different approaches to characterize the structure of Mo_5N_6 along with some results related to the catalytic water-gas shift reaction [4].

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[3] R. Marchand, F. Tessier, F.J. DiSalvo, J. Mater. Chem. 1999, 9, 297.
[4] K. Guy, F. Tessier, S. Cordier, H. Kaper, F. Grasset, N. Dumait, M. Nishio, Y. Matsushita, Y. Matsui, T. Takei, D. Lechevalier, C. Tardivat, T. Uchikoshi, N. Ohashi, Chem. Mater. 2020, 32, 6026.

Venue: B2-41 Classroom, B2 Building, Kofu Campus

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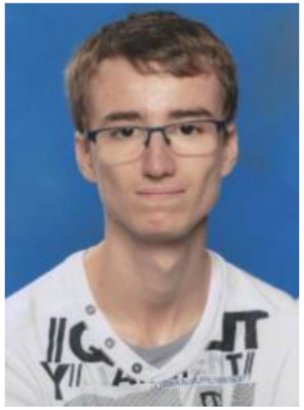

Transition metal nitrides and carbide syntheses from metallic clusters: applications to the Water-Gas Shift (WGS) reaction

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The water gas-shift (WGS) reaction ($H_2O + CO \rightarrow CO_2 + H_2$) is used in non-stationary fuel cells to transform toxic carbon monoxide (CO) for the cell membrane into CO_2. In addition, it produces hydrogen (H_2) from water vapor, useful for the operation of the fuel cell. Currently, this reaction is catalyzed by noble metals, such as platinum. In recent years, there is a renewed interest in finding alternatives to the very expensive and rare noble metals listed as critical raw materials [1]. Several groups have studied the synthesis of new cost-efficient catalysts, among them transition metal nitrides [2].

We report the synthesis of molybdenum nitrides and carbide (Mo_2C, Mo_2N and Mo_5N_6) [3] and other nitrides such as CrN and Ta_3N_5. These compounds were characterized (XRD, BET, SEM..) and evaluated as catalysts for the WGS reaction.

References

[1] Ebrahimi, P., Kumar, A. & Khraisheh, M. A review of recent advances in water-gas shift catalysis for hydrogen production. Emergent Mater. 3 (2020) 881–917.

[2] Hargreaves, J. S. J. Heterogeneous catalysis with metal nitrides. Coord. Chem. Rev. 257 (2013) 2015-2031.

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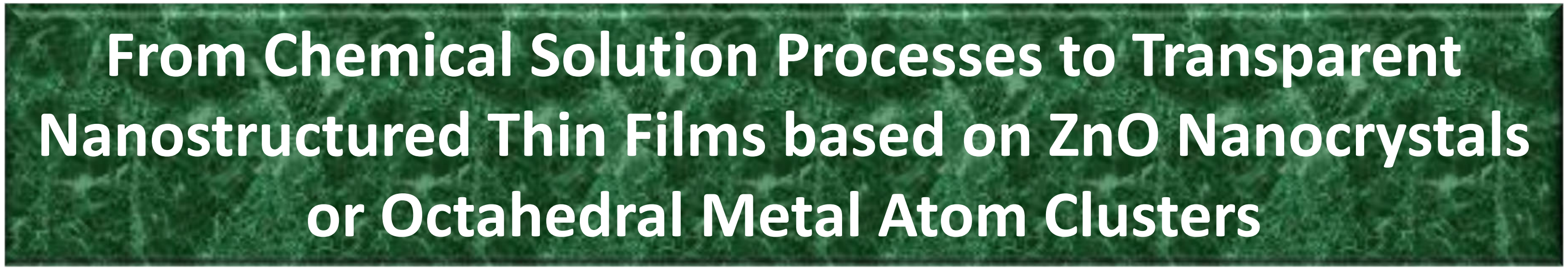

Dr. Fabien Grasset

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Transparent thin films or coatings, with thickness ranging from nanometres to micrometres, are playing an important role in daily life. Recently, the demand of robust, low cost and friendly-environmental functional nanocomposite thin films with high transparency for applications is strongly increasing. Moreover, the use of chemical solution disposition (CSD) processes is highly desirable in order to reduce the cost and waste and that can enable fabrication method for flexible devices. This presentation will summarise our works on the synthesis of functional nanostructured or nanocomposite thin films based on ZnO nanocrystals (NCs) or metal atom clusters (MC) by CSD processes (spin-coating, dip-coating or electrophoretic deposition (EPD)).[1-5] We will demonstrate that CSD processing of inorganic nanocolloidal solutions is highly flexible in terms of precursor composition, targeted substrate and coating procedures at ambient pressures, and thus can be complementary of physical-based deposition routes while providing materials with matching or even superior properties. The first part will focus on colloidal ZnO solutions and particularly their use as negative tone photoresists for direct writing of functional nano-microstructures by deep-UV photolithography.[1] The second part will be devoted on octahedral MC and highly transparent thin films in the visible.[2] Transparent films with prominent photoactive or antibacterial properties were obtained by using specific Mo_6 MC whereas UV and NIR filters were realised by using Ta_6 and Nb_6 MC.[3-4] We will particularly emphasise that the EPD process appears a performant CSD strategy to fabricate highly transparent and coloured nanocomposite thin films for optical, biological and energy applications.[5]

[1] Q. Kirscher et al., Deep-UV laser direct writing of photoluminescent ZnO submicron patterns: an example of nanoarchitectonics concept, Sci. Technol. Adv. Mater., 2022, 23(1), 535. 2) N.T.K. Nguyen et al., A review on functional nanoarchitectonics nanocomposites based on octahedral metal atom clusters (Nb_6, Mo_6, Ta_6, W_6, Re_6): inorganic 0D and 2D powders and films, Sci. Technol. Adv. Mater., 2022, 23(1), 547. 3) K. Kirakci et al., Electrophoretically deposited layers of octahedral molybdenum cluster complexes: a promising coating for mitigation of pathogenic bacterial biofilms under blue light. ACS Appl Mater Interfaces, 2020, 12(47), 52492. 4) C. Lebastard et al., High performance $\{Nb_5TaX_{12}\}$@PVP (X = Cl, Br) cluster-based nanocomposites coatings for solar glazing applications. Sci. Technol. Adv. Mater., 2022, 23(1), 446. 5) N.T.K. Nguyen et al., Extended study on electrophoretic deposition process of inorganic octahedral metal clusters: Advanced multifunctional transparent nanocomposite thin films, Bull. Soc. Chem. Jpn., 2018, 91, 1763.

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Exploring New Materials through Supervised Machine Learning and Generative Model-Based Approaches

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Our research focuses on solid-phase chemistry, utilizing thermodynamic modeling and electronic structure calculations, with a specific emphasis on materials like hydrogen-absorbing intermetallic compounds. We predict phase equilibria and analyze crystal lattice vibrational properties to assess mechanical stability. Recently, we have been employing high-throughput DFT and machine learning algorithms to discover innovative materials, particularly for applications in thermoelectricity and energy storage.

In this presentation, I will focus examples of material discovery, including the prediction of new compositions of known phases via supervised learning and the generation of novel crystal structures through generative algorithms.

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