FKKT | UNIVERZA V LJUBLJANI
Fakulteta za kemijo in kemijsko tehnologijo

VABILO NA PREDAVANJE
V OKVIRU DOKTORSKEGA ŠTUDIJA
KEMIJSKE ZNANOSTI / INVITATION TO THE
LECTURE WITHIN DOCTORAL PROGRAMME IN
CHEMICAL SCIENCES

Prof. dr. Igor Djerdj

Department of Chemistry
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z naslovom / title:

High-entropy oxides

v sredo, 20. 11. 2024 ob 15. uri
v predavalnici 1 v 1. nadstropju Fakultete za kemijo in kemijsko tehnologijo, Večna pot 113 ***/***
on Wednesday, 20. 11. 2024 at 15.00
in lecture room 1, 1st floor at the Faculty of Chemistry and Chemical Technology, Večna pot 113

Vljudno vabljeni! / Kindly invited!

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Abstract:

A new class of materials with enhanced physical and chemical properties and high potential application are multi-component oxides or high-entropy oxides (HEOs). These entropy-stabilized oxides mostly comprise five or more elemental components in an equimolar ratio, incorporated within a single-phase system. The thermodynamic contribution of configurational entropy in the system of minimally five different components is sufficient to overcome the enthalpy of formation and reduce the Gibbs free energy. In this talk, I will present the potential of nanostructured high–entropy oxides (HEOs) for photocatalytic CO_2 hydrogenation, a process with significant implications for environmental sustainability and energy production. Several cerium–oxide–based rare–earth HEOs with fluorite structures were prepared for UV–light driven photocatalytic CO_2 hydrogenation towards valuable fuels and petrochemical precursors. The cationic composition profoundly influences the selectivity and activity of the HEOs, where the $Ce_{0.2}Zr_{0.2}La_{0.2}Nd_{0.2}Sm_{0.2}O_{2-\delta}$ catalyst showed outstanding CO_2 activation (14.4 $mol_{CO}\, kg_{cat}^{-1}\, h^{-1}$ and 1.27 $mol_{CH3OH}\, kg_{cat}^{-1} h^{-1}$) and high methanol and CO selectivity (7.84 % CH_3OH and 89.26% CO) at ambient conditions with 4–times better performance in comparison to pristine CeO_2. The observed formate–routed mechanism and a surface with high affinity to CO_2 reduction offer insights into the photocatalytic enhancement. In addition, I will also present the application of rare-earth HEOs in photoelectrochemical water splitting for hydrogen generation. The $Ce_{0.2}Zr_{0.2}La_{0.2}Pr_{0.2}Y_{0.2}O_2$ (CZLPY) engender hydrogen in 9.2 $\mu molmg^{-1}$ per hour that is much higher content than for pristine CeO_2 material which amounts to 0.8 $\mu molmg^{-1}$ per hour.