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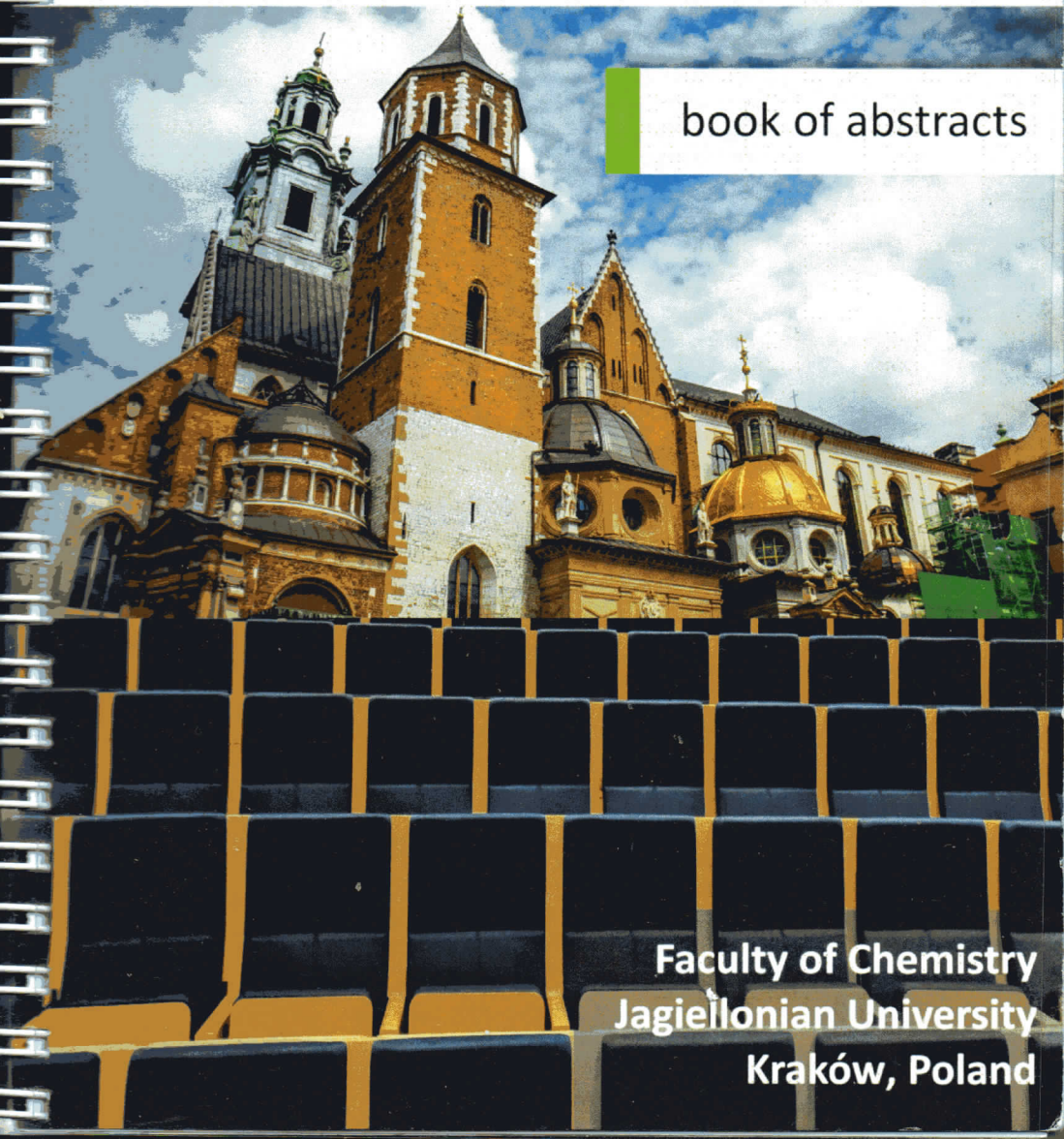

book of abstracts

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KEYNOTE 9

An approach to water splitting based on metal oxide electrodes and polymer electrolyte membranes

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The development of practical devices for direct photoelectrochemical water splitting depends on finding appropriate electrode materials and electrolytes. In comparison with cells based on one photoelectrode, the tandem configuration is especially appropriate because not only the requirements for the electrode materials are less stringent, but also the theoretical solar-to-hydrogen conversion is higher.

Among the electrode materials, those based on earth-abundant elements are particularly interesting. Metal sulfides and oxides are potential candidates and, from the point of view of stability in contact with aqueous solutions, the latter are preferable. Binary oxides have been investigated for more than four decades, while ternary (and more complex) only recently are starting to draw significant attention. Some of the oxides that have been demonstrated to yield significant efficiencies, include Cu_2O and CuO as photocathodes and Fe_2O_3, WO_3 and TiO_2 as photoanodes. While in the case of the photoanodes, the main problem is a poor light harvesting ability, for the photoanodes the main problem is photocorrosion. Ternary oxides, largely unexplored, may offer new opportunities with an adequate trade-off between band gap value and stability. Recent efforts in our laboratory on ternary oxide electrodes are revised first with a focus on photocathodes ($CuFe_2O_4$ or $LaFeO_3$) [1]. Strategies for electrode preparation and modification as well as for obtaining relevant information from photoelectrochemical measurements will be presented.

Another interesting approach that may give rise to more practical and more scalable devices is employing polymer electrolyte membranes (PEM). Preliminary results on a tandem PEM photoelectrochemical cell with CuO and Fe_2O_3 photoelectrodes will be presented including electrode material modification for improved efficiency and stability. The challenges for the implementation of this type of devices is also discussed.

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[1] M.I. Díez-García, R. Gómez, ChemSusChem, 10 (2017) 2457.

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ORAL 8

Computational screening of ternary semiconducting oxides for direct photoelectrochemical water splitting.

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Photoelectrochemical splitting of water has been widely investigated for sustainable production of hydrogen, for use as a fuel or as a high purity reagent. The main obstacles for the development of commercial devices include low solar-to-hydrogen efficiency, expensive electrode materials and fast degradation of prototypes. One attractive way forward is to develop new electrode materials based on earth-abundant elements and to combine them in a tandem cell. In principle, metal oxides may offer good stability in contact with aqueous solutions, either acidic or alkaline. A significant effort has been done since the 1970s to find photoactive binary oxide electrodes and virtually all the practical candidates have been explored. This is not the case of ternary oxides whose number is over 10,000. Several families can be considered, including delafossites, spinels or perovskites. One way to select in a rational way among all these oxides consists in carrying out computational screening (DFT calculations) to determine band gap values and other optoelectronic properties. This selection is intended to provide the input for further experimental testing. The screening strategy and result illustrating some case examples will be presented.

Although our main objective is the development of new electrode materials for photoelectrochemical water splitting, the first-principles study of photocatalytic materials to be presented has a similar impact in related areas such as that of heterogeneous photocatalysis.

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