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**Wolfson Department of Chemical Engineering Seminar**

**Thursday, December 2nd, 2021 at 13:30**

**Via zoom** [**https://technion.zoom.us/j/97577956516**](https://technion.zoom.us/j/97577956516)

**A Faster Path to Solar Fuels:**

**New Approaches for Highly Efficient Materials for Photoelectrochemical Energy Conversion**

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 To achieve a sustainable society with an energy mix primarily based on solar energy, we need means of storing energy from sunlight as chemical fuels (“solar fuels”) that have up to 100 times higher energy and power densities than the best batteries. Viable, global scale photoelectrochemical (PEC) energy conversion of cheap, abundant resources (such as water and CO2) into solar fuels depends on the progress of semiconducting light absorbers with enhanced carrier transport properties, suitable band edge positions, and stability in direct-semiconductor/electrolyte junctions.

The search has concentrated mainly on metal oxides that offer good chemical stability and are wide-ranging, highly tunable multi-functionalities, unparalleled among other materials classes. However, oxide light absorbers tend to suffer from poor charge transport compared to non-oxide semiconductors (e.g., Si, GaAs) due to the formation of polarons. The good news is that only a fraction of the possible ternary and quaternary oxides (together ~ 105 – 106 combinations) have been studied so far, making it likely that the best materials are still waiting to be discovered. The bad news is two-fold: 1) with an increasing number of elements, designing highly controlled synthesis routes of "semiconductor-grade" (i.e., high phase purity, low concentration of bulk and surface defects) oxides will become more thermodynamically and kinetically challenging,[[1]](#footnote-1) and 2) there are currently no robust and proven strategies to identify promising multi-elemental systems.

To overcome these challenges, high-throughput combinatorial investigations of novel non-equilibrium synthesis-parameter spaces and their various “tuning knobs” are required to enable the synthesis of thermally unstable or thermodynamically metastable compositions setting optimized boundary-conditions platforms to maximize the potential of reaching new chemical-physical spaces with enhanced desired properties.

I will introduce an original high-throughput combinatorial approach for exploring large non-equilibrium synthesis-parameter spaces (e.g., temperature, thickness, chemical reactivity) without changing concentration and stoichiometry. The approach allows for high-resolution observation and analysis; even minor changes in synthesis can have a significant impact on the material properties and performances, as demonstrated by a study of the relationship between the crystal structures, synthesis conditions, and properties over a range of thicknesses of CuBi2O4, an emerging photoabsorber for PEC water splitting that was used as a model multinary material.[[2]](#footnote-2)

Near the end of my talk, I will briefly present my plans and vision for researching heteroanionic[[3]](#footnote-3) metal oxynitride materials for PEC energy conversion.[[4]](#footnote-4) Oxynitrides have shown in ideal cases greatly enhanced transport properties, high performances, and increased stability in aqueous solutions when compared to oxides. However, difficulties in synthesizing "semiconductor-grade" oxynitrides model systems leave many questions unanswered about their physical chemistry mechanisms owing to differences in polarizability, electronegativity, nitrogen, and oxygen anion charge. Innovative breakthroughs in the synthesis of oxynitrides will result in their transformation into disruptive and innovative functional materials capable of addressing next-generation major challenges.

1. Gottesman, R. et al. *Adv. Funct. Mater*. 2020, 1910832. [↑](#footnote-ref-1)
2. Gottesman, R. et al. *Adv. Energy Mater*. 2021, 2003474. [↑](#footnote-ref-2)
3. Kageyama, H. et al. *Nat. Commun*. 2018, 772. [↑](#footnote-ref-3)
4. Skrabalak, S. E. et al. *ACS Appl. Mater. Interfaces* 2021, 13, 36670−36678. [↑](#footnote-ref-4)