Department of Chemistry
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Bar-Ilan University

המחלקה לכימיה
הפקולטה למדעים מדויקים
אוניברסיטת בר־אילן

The Department of Chemistry Weekly Seminar

Wednesday 29/12/21 at 11:00am

A Faster Path to Solar Fuels: New Approaches for Highly Efficient Materials for Photo-electro-chemical 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, and 2) there are currently no robust and proven strategies to identify promising multi-elemental systems.

To overcome these challenges, before exploring different compositions, the first step is to place as the central science novel non-equilibrium synthesis methods by high-throughput combinatorial investigations of synthesis parameter spaces. This would open new avenues for the stabilization of metastable materials, the discovery of new chemical spaces, and obtaining light absorbers with

enhanced properties to study their physical working mechanisms in PEC energy conversion. The knowledge gained from studying various "tuning knobs" of non-equilibrium synthesis methods would be used to create optimized boundary conditions platforms to maximize the potential of exploring polyelemental compositions of light absorbers via data-driven combinatorial studies of materials and devices.

I will introduce an original approach for exploring non-equilibrium synthesis-parameter spaces (e.g., temperature, thickness, chemical reactivity) without changing concentration and stoichiometry by employing together two non-equilibrium synthesis key components: pulsed laser deposition (PLD) and rapid radiative heating. A significant advantage of combining these two components is the ability to conduct a highly reproducible, high-throughput combinatorial synthesis that enables high-resolution observation and analysis. Even minor changes in synthesis can have a significant impact on the material properties, physical working mechanisms, and performances, as demonstrated by studies of the relationship between the synthesis conditions, crystal structures of α-SnWO4, and properties over a range of thicknesses of CuBi2O4, both emerging photoabsorbers for PEC water splitting that were used as model multinary materials.

[1] Gottesman, R. et al. *Adv. Funct. Mater.* 2020, 1910832.
[2] Gottesman, R. et al. *ACS Energy Lett.* Just accepted.
[3] Gottesman, R. et al. *Adv. Energy Mater.* 2021, 2003474

Location: Seminar room 112

Looking forward to seeing you!