Department of Chemistry
Faculty of Exact Sciences
Bar-Ilan University

The Department of Chemistry Weekly Seminar
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Experimental Data-driven Paradigms for Unfolding Complexity in Chemical Systems

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In complex chemical systems, finding a complete crystallographic model that folds all the interatomic correlations using a small set of structural descriptors may not always be feasible or practical. Alternatively, one can take a data-driven approach and measure the relative changes in structural and/or chemical features (e.g., structural correlations, oxidation states). An experimental data-driven approach does not require complete models and enjoys the rapidly evolving machine-learning tool-set, which excel at classifying relational datasets and, if also labeled by an observed property, can provide predictive power that links system's descriptors with observed properties.

I will focus on two types of complexities: *hierarchical* complexity, in which different types of structural or chemical correlations change with the probed correlation length, and e*volutionary* complexity, where the order changes over space and/or time. I will demonstrate how both hierarchical and evolutionary complexity can studied and controlled using a data-driven approach. By looking on Ni-laminated Bulk Metallic Glass as a use case [1] of a complex system, I will show how by treating the data as relational, different aspects of the structural and chemical order, such as chemical-short-range-order, can be directly visualized as a function of position. In a different example [2] I demonstrate an autonomous navigation setup in a complex chemical potential space that will help us to achieve a desired chemical state. In this example, we demonstrate an active reaction control of Cu redox state from real-time feedback from in-situ synchrotron measurements.

While complexity can lead to a lack of control over a chemical system, it is essentially adding tuning knobs that, once isolated, understood and controlled, can unlock new materials with desired functionalities.

[1] Y. Rakita, et al., Mapping Structural Heterogeneity at the Nanoscale with Scanning Nano-structure Electron Microscopy (SNEM), arXiv:2110.03589 (2021).
[2] Y. Rakita, et al., Active reaction control of Cu redox state based on real-time feedback from in situ synchrotron measurements, JACS 142, 18758 (2020). DOI: 10.1021/jacs.0c09418