High-throughput materials discovery with nanomaterial megalibraries

Prof. Chad A Mirkin
Northwestern University

Department of Chemistry and International Institute for Nanotechnology

2145 Sheridan Road, Evanston, IL USA 60208

Email: chadnano@northwestern.edu

Identifying new materials that exhibit desired properties is central to everything we do as a civilization. When one considers all the metal elements in the periodic table, and all combinations of them, an infinite number of possible materials exist. This is particularly true at the nanoscale, where minor changes in size or shape at a fixed chemical composition can dramatically change the material's properties. Therefore, the ability to rapidly synthesize and screen materials with desired properties is needed. Towards that, my group has developed a nanoscale scanning probe lithography approach that, through the deposition of polymeric nanoreactors and thermal annealing, enables the preparation of "megalibraries" of as many as 5 billion positionally encoded nanomaterials with distinct chemistries, including metallic and perovskite nanoparticles. These libraries can be tailored to encompass a wide variety of alloys that are comprised of many different elements with up to four phases and six interfaces. Notably, one megalibrary contains new, well-defined inorganic materials that chemists cumulatively have produced and characterized to date. In addition, we are now developing new high-throughput platforms for structural, catalytic, and optical characterization techniques that match the unprecedented speed of megalibrary synthesis. However, in materials discovery efforts, synthetic capabilities far outpace the ability to extract meaningful data from them. To bridge this gap, we present a machine-learning driven, closed-loop experimental process to guide the synthesis of polyelemental nanomaterials with targeted structural properties. Together, this approach lays the foundation for creating an inflection point in the pace at which we both explore the breadth and discover the capabilities of the "matterverse."