

PROJECT SUMMARY (Approved for Public Release): Chirality is a geometrical property with unifying importance for physics, chemistry, biology, astronomy, and mathematics. Despite the large variety of ceramic materials, their multiple nanoscale forms, and high technological importance, chiral ceramic nanostructures are barely known today. The chirality of nanoceramics, combined with their special mechanical, optical, electronic, chemical, and biological properties, as well as their well-known robustness, will enable a vast array of photonic devices, antibacterial drugs, chiral catalysts, biomedical implants, and biosensors with currently unavailable capabilities. **Realization of the vast potential of chiral ceramics requires simultaneous innovation in both chemical and theoretical methods of materials design. Their concerted advancement and integration represents the main goal of this Vannevar Bush project. Our research effort will lead to the establishment of a framework of synthetic protocols, characteristic properties, computational tools, and translational targets for the hierarchical engineering of chiral metal oxides that can extended to other materials.**

Nanoparticles (NPs) of transition metal oxides coated with amino acids will be used as the basic engineering blocks of chiral ceramic materials. The characteristic scale of chirality in NPs will range from a few angstroms to a few nanometers. Chiral ceramics with nano-, meso-, micro-, and macroscale chirality will be obtained by using the NP self-assembly (SA). Applied mathematics of chirality will help us streamline the hierarchical design of chiral materials. A comprehensive set of multiscale chiral indices, describing the structural characteristics of chiral ceramics, will be established as a foundation for a materials engineering toolbox. Specifically, chirality for different structural levels will be cumulatively enumerated as a vectorial set of parameters denoted as **chi**-measures specific for the scale: angstrom-, nano-, meso-.... We shall demonstrate that **chi**-measures at smaller scale determine the **chi**-measures at higher scale. This biomimetic concept is expected to drastically accelerate the materials engineering process compared to ab initio and other computationally heavy materials design approaches. The dependences of **chi**-measures of the SA structures on those of NPs will be experimentally established, computationally validated and used for materials design for different transition metal oxides. The comprehensive evaluation of chemical, physical, and biological properties of chiral nanoceramics will be carried out. Besides the direct match between **chi**-measures of nanostructured ceramics with target geometry, electrodynamic calculations will guide elaboration of the relationships between **chi**-measures and target function. When needed, we shall also apply machine learning techniques to establish relationships between desirable functions and **chi**-measures.

Long-lasting fundamental and practical impacts are expected to emerge from the diverse optical, magnetic, electronic, catalytic, and biological properties as well as the wide accessibility of chiral nanoceramics. The technological relevance of chiral nanoceramics will be demonstrated by: (a) high-performance photonic devices for use under extreme conditions, and (b) nanoscale inhibitors of pathogenic bacteria. Close collaboration between the PI and DoD laboratories, specifically with the Wright-Patterson Air Force Base (WPAFB) scientists, regarding chiral photonics for the near-infrared (NIR) part of the electromagnetic spectrum is anticipated. Additional outcomes of this project will be education and training of a new generation of defense ready workforce versed in a novel, multi-purpose toolbox for materials engineering comprised of cutting-edge methods of nanochemistry, molecular dynamics, and a diverse array of computational technologies.