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ABSTRACT

We propose a far-reaching program on the scientific understanding and discovery of functional materials with strong first order phase transformations exhibiting multiferroic properties and satisfying conditions of supercompatibility. The technical approach involves the development of advanced mathematical theory that guides materials synthesis and characterization. The research is enabled by recent breakthroughs on the understanding of the hysteresis and reversibility of strong first-order phase transformations which is leading to record-setting materials. The focus of the research is the search for *singular materials*, i.e., materials which at particular compositions, with special, nongeneric relations among material constants, exhibit extraordinary behavior. We propose a) to develop a mathematical theory based on first principles methods for the discovery of singular materials, which accounts for nucleation and microstructure, b) to synthesize new highly reversible magnetic/ferroelectric martensites and low hysteresis shape memory alloys with special focus on the theory-guided development of the hybrid molecular beam epitaxy for this purpose, c) to develop mathematical theory and concepts for exceptionally fast switching of phases, d) to discover flexible oxide ceramics with multimillion cycle repeatability, and e) to investigate the light-induced phase transformation in hard materials. The education of students and postdoctoral fellows will transcend traditional boundaries between mathematics and materials science by educating them to a high level in both areas. Frequent technical exchange between the PI, students and postdocs with DoD laboratory personnel will facilitate rapid transfer of theory, concepts and prototypes of singular materials and devices to DoD personnel.