Center for Computational Mesoscale Materials Science (COMMS, DOE-CMS)

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Abstract: The central goal of COMMS, a Computational Materials Science (CMS) Center established in 2019 and supported the US Department of Energy, Office of Science, Basic Energy Sciences, as part of the Computational Materials Sciences Program, is to develop mesoscale computational models, efficient numerical algorithms for exascale computation, and software validated for quantum and functional materials. For the past four years, the Center has been developing phase-field models and software packages for correlated electronic systems and complex topological structures including coupled polarization dynamics, elastodynamics, and electronic carriers and coupled structural and electronic phase transitions in the presence of both electronic carriers and oxygen vacancies. Built upon the existing accomplishments, the specific efforts of the Center for the next three years will be focused on extending our dynamic phase-field model of coupled structural and electronic carrier dynamics to photon dynamics through the study of the formation and responses of mesoscale structures to external mechanical and electromagnetic fields such as light, constructing a set of novel phase-field models of coupled phase transitions such as metal-insulator transitions, magnetic phase transitions, and superconducting phase transitions to study mesoscale electronic and structural pattern formation and evolution under the influence of lattice strain and chemical doping, deploying the corresponding software modules as well as data-generation and mesostructure characterization tools, and experimentally validating the theory and computational tools through extensive collaborations with experts outside the core team on crystal growth, and experimental characterization of mesoscale structures of quantum and functional materials.