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Inverse problems in complex material design: Applications to non-crystalline solids[1] PARTHAPRATIM BISWAS, The University of Southern Mississippi,USA, DAVID DRABOLD, Ohio University,USA, STEPHEN ELLIOTT, University of Cambridge,UK — The design of complex amorphous materials is one of the fundamental problems in disordered condensed-matter science. While impressive developments of ab-initio simulation methods during the past several decades have brought tremendous success in understanding materials property from micro- to mesoscopic length scales, a major drawback is that they fail to incorporate existing knowledge of the materials in simulation methodologies. Since an essential feature of materials design is the synergy between experiment and theory, a properly developed approach to design materials should be able to exploit all available knowledge of the materials from measured experimental data. In this talk, we will address the design of complex disordered materials as an inverse problem involving experimental data and available empirical information. We show that the problem can be posed as a multi-objective non-convex optimization program, which can be addressed using a number of recently-developed bio-inspired global optimization techniques. In particular, we will discuss how a population-based stochastic search procedure can be used to determine the structure of non-crystalline solids (e.g. *a*-SiH, *a*-SiO_2, amorphous graphene, and Fe and Ni clusters).

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