

Abstract Submitted  
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**Engineering of nanomaterials by following the flow of structural information guided by targeted outcome**<sup>1</sup> VLADAN MLINAR, School of Engineering, Brown University, Providence, RI 02912, USA — A fundamental understanding of materials over multi-length scales – with the aim of designing novel nanomaterials and breakthroughs in modern technology is still pending. On the several-atom scale, it has been possible to explore the range of geometrically possible structures and predict new materials that have targeted physical/mechanical properties. However, the question of using those materials in real sizes and “real world” applications is still open. For larger systems, the structure of a material is represented by so-called structural “motifs” such as composition profile, shape, confining potential, or representative volume elements. Here, I will present a methodology based on generalized information theory, where information is conceived in terms of uncertainty. I will demonstrate a mathematical formalism of how to (i) track the loss of structural information between the atomistic description of the structure and description via structural motifs, and (ii) develop a procedure to find the structural motifs responsible for controlling a targeted physical property. To illustrate validity of the approach, I will discuss the design of nanomaterials for intermediate-band solar cells, and how to engineer optimized nanomaterials that can exceed the light-trapping limit.

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