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Inherent limits on optimization and discovery in physical systems

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HIGHLIGHTS

- Graph-based approach to analyze full and partial representations of physical systems.
- Direct link between a change in the physical system and complexity of the graph.
- Inherent limits to the potential for optimization of a general system.
- Inherent limits to the reconstruction of full system from partial representations.

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ABSTRACT

Topological mapping of a large physical system on a graph, and its decomposition using universal measures are proposed. We find inherent limits to the potential for optimization of a given system and its approximate representations by motifs, and the ability to reconstruct the full system given approximate representations. The approximate representation of the system most suited for optimization may be different from that which most accurately describes the full system.

1. Introduction

In the analysis of any large physical system [1,2], e.g., large molecules [3], nanomaterial heterostructures [4], or complex material microstructures [5,6], *ab inito* calculations are often prohibitively expensive and/or some of the underlying physical principles may not be well understood. Two challenges naturally arise. *If the full system is known*, but its behavior cannot be calculated, there

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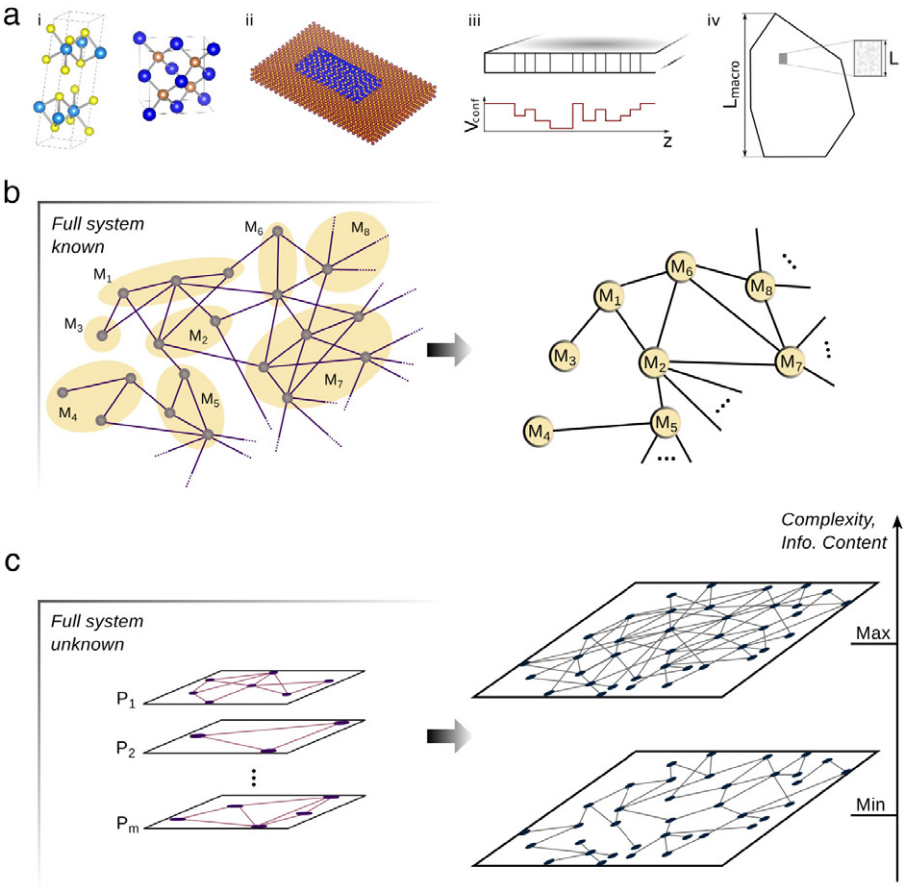

Fig. 1. (a) Description of the structure: (i) on the atomistic level, examples of MoS_2 and InAs; (ii) on the semi-empirical atomistic level ($>10^4$ atoms), where, typically, structural motifs such as the chemical composition and geometry are introduced; example of InSb/GaAs quantum dots; (iii) on the mesoscopic level, where the confining potential is used; example of superlattice; and (iv) on the continuum level, using the concept of a representative volume element (RVE). An RVE plays the role of a mathematical point of continuum field approximating the true material. Note the separation of scales: the microscale d, such as e.g., average size of grain in a given microstructure, the mesoscale L (the size of the RVE), and the macroscale L_{macro}. (b) A physical system is represented via a graph where vertices represent distinguishable units. Every interaction between units is depicted by the link connecting units. The representation of the system via graph can be simplified using motifs, denoted as M_i, where $i = 1, 2, \ldots, 7$. (c) Approximate representations by motifs are known, but the full system remains hidden or unknown to us. Complexity measures and information content are used to determine limits of what can be deduced about the full system.

is a need to group smaller parts of the system into lumped conceptual units (“motifs”); e.g., the concept of a representative volume element in continuum mechanics [5,6]. It becomes necessary to know how best to choose motifs and how much information is lost when the full system is represented by motifs. *If only an approximate representation via motifs and their relationships are known* [2,4,7], it is vital to know how much information can be obtained about the full system.

Perhaps the best way to illustrate this is using structure of materials as an example. The structure is represented via atoms and their positions. This gives the full structural information about the system, including a specific physical property [Fig. 1(a)]. For several-atom systems, the geometrically possible structures and chemical bonds are well understood. Thus, it has become possible to predict new materials on this scale that have targeted physical/mechanical properties (the field of materials informatics) [8,9].