

Materials Science Program Seminar

“Chemical Frustration: Lessons on Materials Design from Complex Intermetallics”

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Time: 4:00 PM - Seminar in Rm. 265 Materials Science and Engineering Building

Host: Prof. Paul Voyles, Materials Science and Engineering Department

ABSTRACT:

Intermetallic phases comprise a domain of compounds with immense diversity both in terms of structural features and physical properties. A limiting factor in developing new intermetallic materials for specific applications is our inability to guide or control their crystal structures. A common theme emerging in the study of the most complex intermetallic phases points toward a possible conceptual framework for approaching such control: structural complexity is increasing being linked to the coexistence of, or competition between, incompatible modes of bonding or packing. We refer to this tension as chemical frustration, to stress an analogy with the origins of complicated magnetic phenomena. In this talk, we will present a theoretical approach to examining one form of tension that can occur in intermetallics: between the dictates of the electronic and atomic size factors occurring within the coordination polyhedra of intermetallic phases. This approach draws on DFT-calibrated Hückel calculations, whose combination of accuracy and transparency provides a simple bridge between DFT results and the experimental parameters adjustable during synthesis. We will show how this theoretical approach yields predictions of ways that frustration can be modulated in synthetic experiments.

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