In the middle of the last century such luminaries as Hume-Rothery, Engle and Brewer, to name but a few, predicted that the coming of electronic structure methods would radically alter our understanding of metallurgical phenomena. Particularly important would be new insights enabling predictions as to the effects of subtle compositional changes on properties mediated at the electronic level, such as phase stability, elastic response, and certain fracture and deformation properties. However, more than fifty years later, our ability to predict compositional effects is largely unchanged by the tremendous advances in electronic structure methods and computational platforms.

It is worth noting, though, that over a similar time period, chemical sciences have been transformed by formalisms gained from electronic structure theory and associated computational methods. Specifically, these formalisms allow us to predict the effects of chemical changes to the properties of molecules and many solids. Among the important components of this formalism are heuristically based theories and concepts, such as: frontier orbitals theory, the Hammond postulate, and chemical functionality. Though all chemists know these foundational concepts relating electronic structure to chemical properties, they are virtually unknown to the physical metallurgist, why?

My belief is that unlike chemistry, where the development of computational methods and a conceptually based framework proceeded in a parallel and synergistic fashion, in the case of metallurgical problems, our expanding computational abilities did not promote or encourage an improved conceptual basis. For example consider the structure and stability of the transition metals. Employing a laptop computer and any one of a number of DFT codes, it is possible to calculate with high accuracy the structure, lattice constant, and elastic properties for most of the transition metals, yet a simple bonding explanation as to why one structure is preferred relative to another remains elusive.

Many distinguished chemists and physicists, including Pauling, Slater, Hoffman and Goddard have commented on the apparent difficulty involved in developing a rationale from which to explain transition metal structure and stability. Though unintended, these well-documented comments have reinforced a common (and I believe widely held) belief that the metallic environment is intrinsically different from that of organics or coordination compounds where chemical fundamentals have proved so valuable—and it is this fact that accounts for our inability to describe metallic structure with simple chemical (bonding) arguments.

In this presentation I will take on the problem of transition metal structure and stability, showing that frontier orbital theory in combination with a basic understanding of the charge density topology of the common transition metal structures (BCC, FCC and HCP) is all that is needed to provide a simple explanation of transition metal phase stability. Illuminating the transition metal structure problem using fundamental chemical principles will go a long way to demonstrating the fallacy of the metallic bond as special myth; and hopefully encourage more chemically based research into the relationships between electronic structure and technologically important metallurgical properties.

Monday, May 18, 2015
4:00 P.M.
2033 Young Hall