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ORIGINS OF MODULATED STRUCTURES

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It is almost always a (pleasant) surprise when a new modulated structure is encountered. This element of surprise points to the need for predictive concepts for understand the origins of incommensurability. In this presentation, we will consider a series of case studies illustrating how modulations can arise from chemical bonding factors. We will begin with a brief overview of charge density waves and Fermi surface nesting as one classic scenario involving mismatches between the periodicities of the atoms and the valence electrons. This will be followed by more recent work illustrating other ways in which incommensurability can be staged: (1) conflicts between the structural preferences of atomic size and electrostatics in the stuffed CoSn series, (2) chemical pressure effects within and between sublattices in the CaPd5 structure, and (3) the interaction between preferred electron counts and chemical pressure effects in a variety of intermetallic phases. As we go through these examples, theoretical and conceptual tools will be introduced that I have found to be useful in understanding such phenomena: the 18-n rule, chemical pressure analysis, and chemical pressure quadrupoles. Common themes will also be identified from the case studies examined, such as the presence of degrees of freedom in a crystal structure than can easily be decoupled from the average structure.