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Novel Visualization of Crystal Structure and Energetics

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ABSTRACT

I am a firm believer in the idea that you have to have the right tool for the right job. And that good tools are inherently community resources. It has been my delight to be a toolmaker and designer in the area of molecular visualization for the past 15 years. In this presentation I will discuss some of my favorite visualizations developed for Jmol over that time, with a focus on the area of solid-state physics and crystal structure. We will take a look at visualization of structure, energy, and symmetry. We will see how a simple accidental switch from a minus to a plus sign completely changes the perspective on close contacts, how solid-state phase transitionscan be visualized as subtle changes in symmetric normal modes, and how the elegant use of "[3 + n]D" symmetry allows the description and visualization of incommensurately modulated structures in a variety of colorful and dynamic ways. We'll see how reciprocal lattices and Brillouin zones can be interactively constructed and explored by students and professionals alike.

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