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Structural properties of kagome-layered crystals

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Recently, a family of kagome metals, AV3Sb5, has been synthesized and found to display superconductivity at low temperatures. Before the onset of superconductivity, a new phase appears at which the material seems to undergo a structural transition which causes the unit cell to double in size. Evidence has been found suggesting that this phase transition is not just a normal structural transition, but that the electronic degrees of freedom are playing an important role, such that this phase has been called Charge Density Wave (CDW). There's a long history of studies surrounding the CDW and its relation to Fermi surface nesting, but the microscopic nature of the order parameter is still under debate.

A kagome-layered structure can be hosted in a number of different materials. A class of them which have received a lot of attention lately, are the shandites A3M2Ch2. In this presentation, we display a symmetry analysis and some first-principles simulations, to investigate if any of the shandites could host a CDW phase like the kagome metals. This would help further our understanding of the nature of the order parameter for a CDW transitions.

Field of study

Quantum Physics

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