



# XI Workshop on Novel Methods for Electronic Structure Calculations

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## Symmetry-obstructed Peierls transition in a topological semimetal

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In many quantum materials, the properties of interest emerge from the interplay between electronic and structural instabilities. A textbook example is the Peierls transition in one-dimensional systems, where a reduction in translational symmetry—driven by the energy gain from associated electronic reconstruction—yields a metal-to-insulator transition. In this talk, we will consider the case of  $\text{PtBi}_2$ , a polar compound whose structure derives from a centrosymmetric phase with larger translational symmetry. Through first-principles calculations, we will show that these two phases are connected by a metal-to-semimetal transition that, similar to the Peierls transition, is driven by an attempt to open a gap in the electronic structure.

In  $\text{PtBi}_2$ , however, this gap fails to fully develop due to constraints imposed by the symmetry of the underlying crystal distortion. Our results not only help us understand the origin of the nontrivial topology in this compound but also illustrate how the Peierls transition can be enriched in higher dimensions through the preservation of additional symmetries.