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Berry Curvature and Multiband formation in TaP

Berry phase is a quantity that describes how a global phase accumulates as some complex vector is carried around a closed loop in a complex vector space.
Berry phase and related concept, usually provide a unified framework for describing many fundamental properties of electrons in solids. By this we imply from electric polarization to quantized effects in topological materials. Tantalum Phosphide (TaP), a verified weyl semi-metal is a suitable candidate in Berryology in that many of its its intrinsic properties remain unknown. In this work, the authors will employ a class of mathematical methods that are connected to the specific geometric phases in TaP. These so called phases, are the Berry phases and they have significant roles in the band theory of electrons in TaP. We shall employ the state-of-the-art \textit{ab initio} methods as implemented in {\sc Siesta} method. The authors herein will introduce the concept of the Berry phase and explain how it enters into the quantum-mechanical band theory of electrons in crystals. As a matter of fact, we will also discuss its application to the normal adiabatic dynamics of finite quantum systems.

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