

First principle calculations of g-factor and topological phase transitions in topological materials under external magnetic field

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Zeeman effect plays a crucial role in determine the behavior of topological semimetals under magnetic field. In the present talk, I will introduce the first principle method to calculate the g-factor at general k-points in the Brillouin Zone for materials with strong spin orbit coupling. I will first demonstrate that the g-factor for the particular Bloch states comes from the screening effect of the high-energy bands and it depends on the form of the low energy effective model. Then I will introduce the main results obtained by density functional theory for the g-factors of the selected topological semimetals and the possible topological phase transitions under the magnetic field.