Effect of spin-orbit coupling on the high harmonics from the topological Dirac semimetal Na<sub>3</sub>Bi

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## Abstract:

In this work, we performed extensive first-principles simulations of high-harmonic generation in the topological Diract semimetal Na<sub>3</sub>Bi using a time-dependent density functional theory framework, focusing on the effect of spin-orbit coupling (SOC) on the harmonic response. We also derived a general analytical model describing the microscopic mechanism of strong-field dynamics in presence of spin-orbit coupling, starting from a locally U(1)xSU(2) gauge-invariant Hamiltonian. Our results reveal that SOC: (i) affects the strong-field ionization by modifying the bandstructure of Na<sub>3</sub>Bi, (ii) modifies the electron velocity, making each spin channel to react differently to the pump laser field, (iii) changes the emission timing of the emitted harmonics. Moreover, we show that the SOC affects the harmonic emission by directly coupling the charge current to the spin currents, paving the way to the high-harmonic spectroscopy of spin currents in solids.



Figure: High-harmonic generation from Na<sub>3</sub>Bi with and without SOC for a linearly-polarized laser field.

## **Reference:**

[1] N. Tancogne-Dejean, F.G. Eich, A. Rubio. *Effect of spin-orbit coupling on the high harmonics from the topological Dirac semimetal Na*<sub>3</sub>*Bi*. Submitted (2021)