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Lifshitz-type metal-to-insulator transition via strong relativistic renormalization in $\mathbf{NaOsO_3}$ BONGJAE KIM, PEITAO LIU, ZEYNEP ERGÖNENC, University of Vienna, Faculty of Physics, Computational Materials Physics, ALESSANDRO TOSCHI, Institut für Festkörperphysik, Technische Universität Wien, SERGII KHMELEVSKYI, University of Vienna, Faculty of Physics, Computational Materials Physics and Department of Physics, Budapest University of Technology and Economics, CESARE FRANCHINI, University of Vienna, Faculty of Physics, Computational Materials Physics — Using *ab initio* band structure methods in the framework of density functional theory (DFT), we study the mechanism responsible for the metal-to-insulator transition (MIT) in the $5d$ oxide $NaOsO_3$ and reinterpret its previously proposed Slater nature. We show that spin-orbit coupling (SOC) causes a strong relativistic renormalization of the electronic correlation that moves the system to a weakly interacting itinerant limit, where the physics of itinerant magnetism prevails. This is the opposite effect as compared to the widely studied iridates, where SOC drives the formation of a relativistic Mott state. By mapping the magnetically constrained non-collinear DFT calculation using spin-fluctuation theory, we explain the MIT of the system in connection with the anomalies observed in the experimental resistivity curve. We show that the continuous MIT is associated to the progressive disappearance of electron and hole pockets in the Fermi surface, typical of a Lifshitz-type MIT, and is mediated by spin-fluctuations. We discuss the inconsistencies of a pure Slater interpretation and propose that $NaOsO_3$ should be classify as a magnetically-driven relativistic Lifshitz insulator.

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