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First-principles evidence of Slater-type metal-to-insulator transition in NaOsO3 BONGJAE KIM, ZEYNEP ERGONENC, CESARE FRANCHINI, Faculty of Physics and Center for Computational Materials Science, University of Vienna — $NaOsO_3$ is thought to be the first example of a three-dimensional Slater insulator where the metal-to-insulator transition (MIT) is driven by the emergence of the (antiferro)magnetism in the system. This picture is fundamentally different from the most widely known Mott-Hubbard (MH) insulators for which the opening of the gap is due to electron correlation. Even though there are experimental evidences for the Slater-type sate in $NaOsO_3$ such as the continuous character of the transition and the simultaneous onset of the magnetic and insulating regime at the same temperature (T_{MIT}=T_N), no direct and unambiguous indication has been provided by the theory side. Based on *ab initio* band structure methods, we have studied the origin of the MIT in $NaOsO_3$ and found that the MIT is predominantly driven by magnetism, and only marginally dependent on electronic correlation. A direct comparison between $NaOsO_3$ and other typical MH oxides allows us to analyze and interpret the distinct role of magnetism and the electronic correlation in favoring Slater- or MH-type states. Finally, fingerprints of the Slater behaviour are found in the optical response, that we have computed within a model Bethe-Salpeter scheme.

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