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Quantum Monte Carlo simulations of Ti4O7 Magnéli phase ANOUAR BENALI, Argonne Natl Lab, LUKE SHULENBURGER, Sandia National Laboratories, JARON KROGEL, Oak Ridge National Laboratory, XIAOLIANG ZHONG, Argonne National Laboratory, PAUL KENT, Oak Ridge National Laboratory, OLLE HEINONEN, Argonne National Laboratory — Ti4O7 is ubiquitous in Ti-oxides. It has been extensively studied, both experimentally and theoretically in the past decades using multiple levels of theories, resulting in multiple diverse results. The latest DFT+SIC methods and state of the art HSE06 hybrid functionals even propose a new anti-ferromagnetic state at low temperature. Using Quantum Monte Carlo (QMC), as implemented in the QMCPACK simulation package, we investigated the electronic and magnetic properties of Ti4O7 at low (120K) and high (298K) temperatures and at different magnetic states. This research used resources of the Argonne Leadership Computing Facility at Argonne National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357. L.S, J.K and P.K were supported through Predictive Theory and Modeling for Materials and Chemical Science program by the Office of Basic Energy Sciences (BES), Department of Energy (DOE) Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-AC04-94AL85000.

Anouar Benali
Argonne National Laboratory

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