

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Quantum Monte Carlo of ThO₂¹ SHUMING HU, LUBOS MITAS, Physics Department, North Carolina State University — Thorium dioxide solid is a unique optical and heat-resistant actinide material with large gap and cohesion. It is a diamagnet, unlike a number of other similar actinide oxides. We investigate the electronic structure of ThO₂ using Density Functional Theory (DFT) and quantum Monte Carlo (QMC) methods. We adopt Stuttgart RLC and RSC effective core potentials (pseudopotentials) for the Th atom. In the DFT calculations, some of the properties are verified in all-electron calculations using the FLAPW techniques. Using the fixed-node diffusion Monte Carlo we calculate the ground state and several excited states from which we estimate the cohesion and the band gap. Simulation cells of several sizes are used to estimate/reduce the finite size effects. We compare the QMC results with recent DFT calculations with several types of functionals which include hybrids such as PBE0 and HSE. Insights from QMC calculations give us understanding of the correlations beyond the DFT approaches and pave the way for accurate electronic structure calculations of other actinide materials.

¹Supported by DOE and NSF

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Date submitted: 08 Nov 2011

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