

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Zirconia and its allotropes; A Quantum Monte Carlo study. ANDREA JOKISAARI, Northwestern University, ANOUAR BENALI, HYEONDEOK SHIN, YE LUO, ALEJANDRO LOPEZ BEZANILLA, LAURA RATCLIFF, PETER LITTLEWOOD, OLLE HEINONEN, Argonne National Laboratory — With a high strength and stability at elevated temperatures, Zirconia (zirconium dioxide) is one of the best corrosion-resistant and refractive materials used in metallurgy, and is used in structural ceramics, catalytic converters, oxygen sensors, nuclear industry, and in chemically passivating surfaces. The wide range of applications of ZrO₂ has motivated a large number of electronic structures studies of its known allotropes (monoclinic, tetragonal and cubic). Density Functional Theory has been successful at reproducing some of the fundamental properties of some of the allotropes, but these results remain dependent on the specific combination of exchange-correlation functional and type of pseudopotentials, making any type of structural prediction or defect analysis uncertain. Quantum Monte Carlo (QMC) is a many-body quantum theory solving explicitly the electronic correlations, allowing reproducing and predicting materials properties with a limited number of controlled approximations. In this study, we use QMC to revisit the energetic stability of Zirconia's allotropes and compare our results with those obtained from density functional theory.

Anouar Benali
Argonne National Laboratory

Date submitted: 11 Nov 2016

Electronic form version 1.4