MAR17-2016-007919
C

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Soft Functionals for Hard Matter[1]

VALENTINO R. COOPER, SIMUCK F. YUK, JARON T. KROGEL, Oak Ridge National Laboratory

Theory and computation are critical to the materials discovery process. While density functional theory (DFT) has become the standard for predicting materials properties, it is often plagued by inaccuracies in the underlying exchange-correlation functionals. Using high-throughput DFT calculations we explore the accuracy of various exchange-correlation functionals for modeling the structural and thermodynamic properties of a wide range of complex oxides. In particular, we examine the feasibility of using the nonlocal van der Waals density correlation functional with C09 exchange (C09x), which was designed for sparsely packed soft matter, for investigating the properties of hard matter like bulk oxides. Preliminary results show unprecedented performance for some prototypical bulk ferroelectrics, which can be correlated with similarities between C09x and PBEsol. This effort lays the groundwork for understanding how these soft functionals can be employed as general purpose functionals for studying a wide range of materials where strong internal bonds and nonlocal interactions coexist.

[1]Research was sponsored by the US DOE, Office of Science, BES, MSED and Early Career Research Programs and used resources at NERSC.