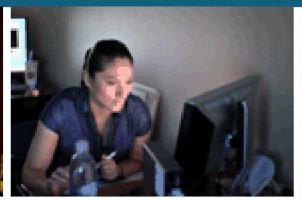
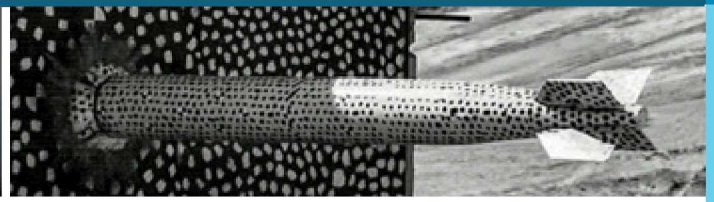
SAND2019-3780PE

Description of a solid using quantum Monte Carlo methods





PRESENTED BY

Principal Investigator/Lab: Luke Shulenburger

Platform/Campaign ID: atcc6-242k
Code Name:
Program: SC
Usage: 1

SNL R&A # (SAND, PR):

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ATCC6-242k Explored Methods For Strongly Correlated Materials

Background Description:

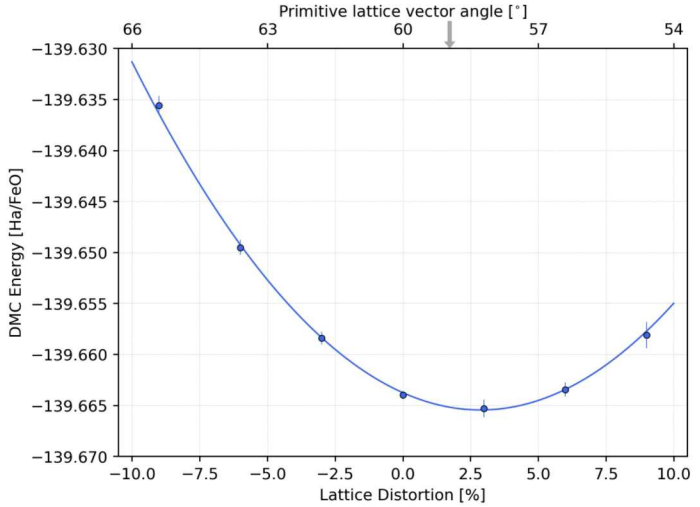
- Performed high-accuracy Quantum Monte Carlo (QMC) calculations on antiferromagnetic iron oxide
- QMC is useful for describing systems with highly localized electronic states, challenging for more common mean field methods

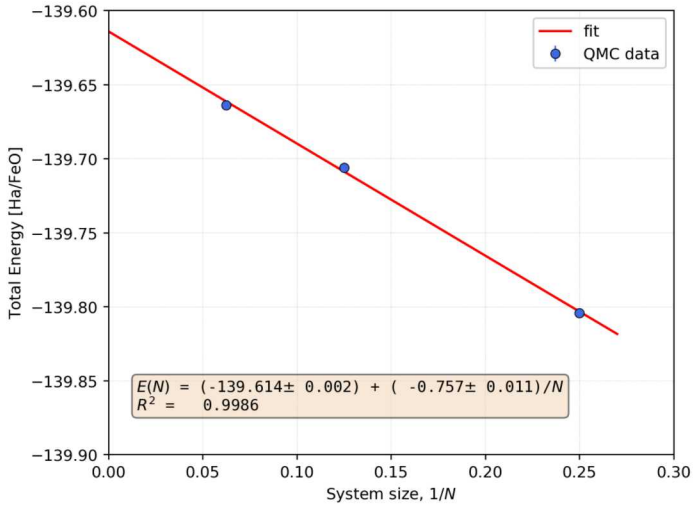
Potential Consequences/Issues:

- QMC methods are much more (~10-100x) computationally expensive than mean-field methods

Resolution/Impact:

- Demonstrated accuracy and feasibility of method with system scaling calculations





Trinity enabled highly accurate QMC calculations for a large strongly correlated material