Centre for High Performance Computing 2019 National Conference



Contribution ID: 108 Type: Talk

Predicting Thermodynamic Properties of Ionic Liquids—from Molecular Simulation to Machine Learning

Monday, 2 December 2019 14:10 (20 minutes)

Supported Student

Primary author: Dr VENTER, Gerhard (University of Cape Town)

Co-authors: WILSON, Tayla; CARROLL, Lenard (University of Cape Town)

Presenter: Dr VENTER, Gerhard (University of Cape Town)

Session Classification: HPC Applications

Track Classification: Computational Chemistry