

Discussion Session I

Wednesday, 5 November 2014 14:25 (1:15)

Content

on electronic structure computations and the development of MD potentials.

Questions: 1a: What is the role of electronic excited states and how can effects of electronic excitation be included in the models and data?

1b: Are we satisfied with present strategies for the development of MD potentials from electronic structure calculations?

Summary

Session Classification : Session