

Contribution ID : 940

Type : **not specified**

Car and Parrinello meet Green and Kubo: simulating atomic heat transport from equilibrium ab initio molecular dynamics

Friday, 13 January 2017 16:10 (0:30)

Content

Summary

Presenter(s) : S. BARONI (SISSA, Trieste)

Session Classification : Session: Temperature and phonon effects, thermal transport