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18th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods | (smr 3101)

Friday 13 January 2017

Session: Temperature and phonon effects, thermal transport - Budinich Lecture Hall (LB)
(16:05-17:40)

time	title	presenter
16:05	Introduction to the session	
16:10	Car and Parrinello meet Green and Kubo: simulating atomic heat transport from equilibrium ab initio molecular dynamics	S. BARONI
16:40	Non-locality in lattice thermal conductivity	P. ALLEN
17:10	One-shot calculation of temperature-dependent optical spectra and phonon-induced band-gap renormalization	F. GIUSTINO