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20th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods | (smr 3554)

Wednesday 24 February 2021

Contributed talks - Online (14:16-15:50)

Chair: Shobhana NARASIMHAN (JNCASR, India)

The talk will last for 18 minutes, with further 3 minutes for questions.

time	title	presenter
14:16	Investigation of one-dimensional materials	HADEEL MOUSTAFA
14:37	Ab initio calculation of the shift photocurrent by Wannier interpolation	JULEN IBANEZ AZPIROZ
14:58	Materials discovery for biomedical applications: from machine learning and first principles calculations to finite elements	CAETANO RODRIGUES MIRANDA
15:19	Lattice thermal conductivity of highly anharmonic materials: Beyond the Boltzmann transport approach	DJORDJE DANGIC
15:40	Coffee break	