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Joint ICTP-IAEA School and Workshop on Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments | (smr 3197)

Wednesday 18 April 2018

Session 3c - Nuclear dynamics in materials II - Budinich Lecture Hall (LB) (14:00-16:00)

- Conveners: T. Oda

time	title	presenter
14:00	Estimation of atomistic properties using computer simulations and UQ methods	VON TOUSSAINT, Udo
14:35	Multiscale QM/MM simulation of chemo-mechanical processes in materials: from crack propagation in silicon to dislocation motion in tungsten	KERMODE, James R.
15:10	Quadratic to higher-order Jahn-Teller coupling effects and subfemtosecond proton dynamics in tetrahedral systems	MONDAL, Tanmoy
15:30	Coffee break	