



# Table of contents

Monday 29 January 2018 .....	1
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# MaX Conference on the Materials Design Ecosystem at the Exascale: High-Performance and High-Throughput Computing | (smr 3161)

## Monday 29 January 2018

**Advances in Electronic Structure I: Frontiers for technologies - Budinich Lecture Hall (LB)**  
**(11:00-14:45)**

time	title	presenter
11:00	Ab-initio Green-Kubo Simulation of Thermal Transport in Liquids and Glasses: A Challenge to Theoretical Physics and to HPC Technology	S. BARONI
11:25	On the Enhanced Thermal Transport Properties of Graphene Nanofluids	P. ORDEJON
11:50	New Energy Materials from Data-driven Computations of Transport Properties	B. KOZINSKY
12:15	Understanding Water/Solid Functional Interfaces for Photocatalysis and Electrochemical Applications	M. FERNANDEZ-SERRA
12:40	Lunch break	