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# College on Multiscale Computational Modeling of Materials for Energy Applications | (smr 2874)

## Monday 04 July 2016

### Session 2 - AGH (Kastler Lecture Hall) (13:45-17:00)

#### *From ab-initio to classical molecular dynamics*

time	title	presenter
13:45	Understanding renewable energy materials by combining first principles modeling and experimental characterization	CHAN, Maria
14:45	Computational Studies of Novel Solar Energy Materials: Defects and Inverse Design	GONG, Xingao
15:45	Coffee break	
16:00	Computational design of novel sustainable catalysts for fuel cell technologies	FABRIS, Stefano