

# Theory & Modelling of Materials in Extreme Environments

25-28<sup>th</sup> September:

The Garden Room, The Cosener's House, Abingdon, Oxfordshire

**DAY 1: Sunday 25<sup>th</sup> September**

17:00 – 19:00	ARRIVAL & DINNER
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**DAY 2: Monday 26<sup>th</sup> September**

09:00 – 09:10	Mike Finnis	Welcome and introduction
	<b>SESSION 1: Mechanics</b>	
09:10 – 09:55	Nik Petrinic	<i>Dynamic Adaptive Recursive Concurrent Multi-scale Simulations of the Response of Hybrid Lightweight Systems to Impact Loading</i>
09:55 – 10:15	Vassili Vorontsov	<i>Development of Multi-scale Modelling Tools for Design and Optimisation of Super-alloys for High-temperature Applications</i>
10:15 – 10:35	Zhen Zhang	<i>Importance of Micro Texture in Adiabatic Shear Bands in Polycrystals</i>
10:35 – 12:05	<b>REFRESHMENTS &amp; POSTERS</b>	
12:05 – 12:50	Kamran Nikbin	<i>Predictive Meso-scale Modelling of Environmental Creep Damage and Cracking of Ceramics under Ultra-high Temperature Conditions</i>
12:50 – 13:10	Peter Brown	<i>Defence Materials Modelling</i>
13:10 – 14:10	<b>LUNCH</b>	
14:10 – 14:55	Daniel Balint	<i>New Advances in Discrete Dislocation Plasticity for Extreme Engineering Environments</i>
	<b>SESSION 2: Lattice models</b>	
14:55 – 15:15	Pui Wai Ma	<i>Spin-lattice Magnetic Molecular Dynamics: Fundamentals and Applications</i>
15:15 – 15:35	Xin Wang	<i>Modelling Microstructure of Materials by Cellular Automata</i>
15:35 – 16:35	<b>REFRESHMENTS &amp; POSTERS</b>	
	<b>SESSION 3: Radiation Damage</b>	
16:35 – 17:20	TBC	
17:20 – 17:40	Andrea Sand	<i>Statistical Laws of Radiation Damage</i>
17:40 – 19:00	<b>GENERAL DISCUSSION / BREAK</b>	
19:00	<b>DINNER</b>	

### **DAY 3: Tuesday 27<sup>th</sup> September**

<b>SESSION 4: High T &amp; P</b>		
09:00 – 09:40	Luc Vandeperre	<i>Challenges and Opportunities with Ultra-high Temperature Ceramics</i>
09:40 – 10:25	Joerg Neugebauer	<i>Modelling Structural Materials in Extreme Environments by Ab-initio-guided Multiscale Simulations</i>
10:25 – 11:30	<b>REFRESHMENTS</b>	
11:30 – 11:50	Umberto Terranova	<i>Structure and Dynamics of Water at the Interface with Mackinawite in Hydrothermal Vents</i>
11:50 – 12:35	Chris Pickard	<i>High Pressure – a Gift to Theory</i>
12:35 – 14:05	<b>GENERAL DISCUSSION / LUNCH</b>	
<b>SESSION 5: Earth Science</b>		
14:05 – 14:50	Dario Alfe	<i>Earth's Core-Mantle Equilibrium and a Heat Sink at the Core Mantle Boundary</i>
14:50 – 15:10	Hang Cui	<i>The Reaction of MgO with Iron in the Deep Earth</i>
15:10 – 15:30	Bing Xiao	<i>Vaporisation of MgSiO<sub>3</sub></i>
15:30 – 16:30	<b>REFRESHMENTS / POSTER SESSION</b>	
<b>SESSION 6: Fewer Dimensions</b>		
16:30 – 17:15	Wolfgang Windl	<i>Novel Approaches to Validated Modelling of Point Defects and Surface Processes</i>
17:15 – 17:35	Ji Chen	<i>Two Dimensional Ice from First Principles</i>
17:35 – 17:55	Samuel Murphy	<i>Electronically Driven Ultrafast Phase Transformations in Tungsten Nanofilms</i>
17:55 – 19:00	<b>GENERAL DISCUSSION/BREAK</b>	
19:00	<b>DINNER</b>	

### **DAY 4: Wednesday 28<sup>th</sup> September**

<b>SESSION 7: Composites</b>		
09:00 – 09:45	Frank Zok	<i>Probing Ceramic Composites under Extreme Environments</i>
09:45 – 10:05	Frank Abdi	<i>Foreign Object Damage (FOD) and Fatigue Validation Prediction with Electrical Resistance Strategy</i>
10:05 – 10:25	Frank Abdi	<i>Mode I-II Crack Growth Resistance in Ceramic Matrix Composites (CMCs)</i>
10:25 – 11:00	<b>REFRESHMENTS</b>	
11:00 – 11:45	TA Parthasarathy	<i>A Multi-physics Modelling Approach to Capture Architecture-dependent Effects on the Environmental Degradation of SiC-fibre Reinforced CMCs</i>
11:45 – 12:05	Severin Hofmann	<i>Finite Element Analysis of a Carbon Fibre Reinforced SiC Nozzle under Internal Pressure Load</i>
12:05 – 12:25	Craig Przybyla	<i>Microstructure-sensitive Damage Characterisation / Simulation in Continuous Fibre-reinforced Ceramic Composites</i>
12:25 – 13:05	<b>GENERAL DISCUSSION / BREAK</b>	
13:05	<b>LUNCH &amp; DEPARTURE</b>	