Nanomaterials

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Defect-induced effects in nanomaterials

Following the success of 5 previous symposia, this one is dedicated to further exploring the basic properties and technology of nanomaterials using the controlled introduction of defects through the application of external loads, including ionizing and particle radiation.

Scope:

Solids without defects are impossible to achieve based on thermodynamics. The defects are Janus Bifrons: they can deteriorate the properties of materials and structures, but they can also enhance them with unique and useful properties which are absent in the perfect solids. Due to the wide applications of nanotechnology it is necessary to invest efforts in studying the formation of evolution and defects at the nanoscale The high sensitivity of modern technologies on the submicron scale has promoted the exciting opportunity of developing new advanced materials with reduced dimensionality. This opens new prospects for ion and electron beam applications. Ion tracks and other radiation-induced effects provide a means for controlled synthesis and modification of low-dimensional materials, such as nanoclusters and nanowires, allowing for efficient nano- and optoelectronic devices. Defect behavior in nanomaterials and nanostructures in its turn has often been found to differ substantially from that observed in bulk materials. Recent work has demonstrated spectacular optical and magnetic effects due to deliberately created defects or radiation-induced transformation of nanomaterials as well as radiation-induced displacements in low-dimensional insulators and semiconductors, with numerous potential applications. We plan to discuss how such defects could be introduced controllably, categorized and controlled in nanostructures. Understanding and controlling defect properties and capturing the grain boundary effects in a wide class of advanced nanostructures (novel 2D materials, multiferroics, quantum dots and wires, etc.) could well be a key to breakthroughs in several crucial areas of science and technology. This is the main focus of the symposium. Since a complete and detailed understanding of all of the above is impossible without computational approaches, the latter techniques, including ab initio calculations, will also be favored.

Hot topics to be covered by the symposium:

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- Defects in graphene and other 2D materials
- Swift heavy ion irradiation as the means to tailor nanomaterials
- Effects of grain boundaries and interfaces on the diffusion and transport processes in nanomaterials
- Electronic structure of defects in nanostructures
- Creation, evolution and properties of radiation defects in nanosize materials and heterostructures; the role of interfaces, nonstoichiometry
- Multiscale computer modeling of defect creation and transformation in nanomaterials
- Novel technological processes of micro-, nano- and optoelectronics using defects and radiation effects

No abstract for this day

START AT	SUBJECT	View All	NUM.	ADD

Session 1 : NN

START AT	SUBJECT	View All	NUM.	ADD
09:00	X-ray absorption spectroscopy as a powerful tool for nanoscience		**M.1.1**	☆

Authors : Andris Anspoks, Aleksejs Kuzmins
Affiliations : Institute of Solid State Physics, University of Latvia

Resume : X-ray absorption spectroscopy (XAS) is an element-specific technique that is sensitive to the local electronic and geometric structure around absorbing atoms. As an element-specific method, it is unique for the analysis of dopants and multi-element compounds. It provides information even in cases where diffraction data cannot be obtained, including amorphous materials, liquids and gases. In this talk, I will focus on the possibilities that XAS opens up for nanoscience and defect analysis using X-ray absorption near-edge structure (XANES) and extended X-ray absorption fine structure (EXAFS).

START AT	SUBJECT	NUM.	ADD
09:30	Engineering defect interactions in filamentary valence-change memristive devices towards neuromorphic computing	**M.1.2**	☆
10:00	Impact of structural defects on the electrical and optical properties in Indium Phosphide (InP) material	**M.1.3**	☆
10:15	Investigation of graphene on SiC under neutron irradiation by Raman Spectroscopy	**M.1.4**	☆

START AT	SUBJECT	View All	NUM.	ADD
10:30	*Coffee break*			
	Session 2 : NN			
11:00	Impacts of Interfaces and Element Deficiency on Catalytic Activities: Cases of Bi-based semiconductor systems		**M.2.1**	☆
11:30	The angular overlap approach to ligand field theory - An almost forgotten model with chemical intuition		**M.2.2**	☆
12:00	First-principles calculations of F-centers and iridium impurities in gallium oxide polymorphs.		**M.2.3**	☆
12:15	Tailoring of room temperature ferromagnetism in GaN thin films by ion irradiation: Experimental and First principle-based study		**M.2.4**	☆
12:30	*Lunch*			
14:00	Ion implantation and defect engineering in wide bandgap semiconductor nanostructures		**M.3.1**	☆

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START AT	SUBJECT View All	NUM.	ADD
14:30	High pressure study of yellow luminescence in Be- and C-doped GaN - experimental and theoretical analysis	**M.3.2**	☆
15:00	Calculation of thermoluminescence kinetic parameters of zirconium dioxide ceramics synthesized in a beam of high-energy electron	**M.3.3**	☆
15:15	Spectral properties of YAG doped with europium of various concentration	**M.3.4**	☆
15:30	*Coffee break*		

Session 4 : NN

START AT	SUBJECT	NUM.	ADD
16:00	Experimental and theoretical investigations of local environment of Mn ions in red phosphors	**M.4.1**	☆
16:30	Nanoscale Trap Clusters in Halide Perovskite Semiconductors	**M.4.2**	☆
17:00	Ab initio modelling for predicting new chalcopyrite photovoltaic materials	**M.4.3**	☆

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START AT	SUBJECT View All	NUM.	ADD
17:15	In-plane stress-enhanced grain boundary segregation and interface diffusion in immiscible Cu/W nano-multilayers	**M.4.4**	☆

Poster session : NN

START AT	SUBJECT	NUM.	ADD
17:30	Atomistic Simulations of Defects Production at Epitaxial Graphene on SiC	**M.P.1**	☆
17:30	Simulation of a single-electron device based on endohedral fullerene (KI)@C180	**M.P.2**	☆
17:30	A Study on Reaction Characteristics of Al-based Reactive Material Structures by Introduction of Nano Defects and Nano Interfaces	**M.P.3**	☆
17:30	Characterization of Porous-CdO/Porous-CdS nanocomposite obtaining electrochemical method	**M.P.4**	☆
17:30	Aluminum-magnesium spinel: optical effects of high-energy ion irradiation	**M.P.5**	☆
17:30	The formation and characterization of arsenolite crystallites on GaAs surface	**M.P.6**	☆

START AT	SUBJECT View All	NUM.	ADD
17:30	Statistical analysis of tensile deformation of Al nanowire	**M.P.7**	☆
17:30	Computer simulation of the density of state of alkali halide nanocrystals	**M.P.8**	☆
17:30	Modeling of core-structure and lattice resistance of twinning dislocation in FCC metals	**M.P.10**	☆
17:30	Elucidating the role of surfactants in growth and charge carrier dynamics of Cs4CuSb2Cl12	**M.P.11**	☆
17:30	Calculation of physicochemical properties of alkali halide nanotubes	**M.P.12**	☆
17:30	A role of intrinsic vacancy defects in electronic and optical properties of ?-Ga2O3 crystal. Ab initio LCAO study.	**M.P.14**	☆
17:30	Computational studies of doped and functionalized cellulose-carbon nanocomposite materials	**M.P.15**	☆
17:30	Defect-related luminescence in fast neutron irradiated corundum crystals	**M.P.16**	☆

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START AT	SUBJECT View All	NUM.	ADD
17:30	Study of defect induced effects in REVO4 nanoparticles doped with Ca cations	**M.P.17**	☆
17:30	Structural studies of the Radiation assisted synthesized gallium oxide ceramics	**M.P.18**	☆
17:30	MgAl2O4:Cr3+ - experimental and theoretical analysis of the optical spectra	**M.P.19**	☆
17:30	Determining GaN (non)Luminescent Defect Distribution by Super/Sub-Bandgap Surface Photovoltage Spectroscopy	**M.P.20**	☆
17:30	Effect of radiation on the electrical properties of oxidized porous silicon – reduced graphene oxide hybrid structures	**M.P.21**	☆
17:30	Doping Zinc Oxide Nanoparticles by Magnetic and Nonmagnetic Nanocomposites Using Organic Species for Fast Removal of Industrial	**M.P.22**	☆
17:30	Structural and optical characterization of TiO2 nanocrystalline materials synthesized by different methods.	**M.P.23**	☆

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START AT	SUBJECT View All	NUM.	ADD
17:30	Structure and magnetic properties of Ni-doped tin oxide films	**M.P.25**	☆
17:30	Structural studies of the radiation assisted synthesized gallium oxide ceramics	**M.P.26**	☆
17:30	Radiation induced defects in cerium doped GAGG single crystals induced by swift heavy ions	**M.P.27**	☆
17:30	Luminescence efficiency of YAG:Ce, Gd, Ga ceramics synthesized by radiation assisted method	**M.P.28**	☆
17:30	Preparation and optical properties of K2O-P2O5-MoO3-Bi2O3-KBi(MoO4)2:Eu glass-ceramics	**M.P.29**	☆
17:30	Ag2O-HgCdTe nanocomposite formed by silver ion implantation for multispectral detection	**M.P.30**	☆
17:30	Evolution of free-volume defects in the Cu0.1Ni0.8Co0.2Mn1.9O4 ceramics caused by interphase mass-transfer processes Authors : H. Klym (1), I. Karbovnyk (1,2), A.I. Popov (3) Affiliations : (1) Lviv Polytechnic National University, Lviv, Ukraine (2) Ivan Franko National University of Lviv, Lviv,	**M.P.31**	☆

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Ukraine (3) Institute of Solid State Physics, University of Latvia, Riga, Latvia

Resume : Technologically-modified Cu0.1Ni0.8Co0.2Mn1.9O4 ceramics are widely used as one of the most perspective materials for application as negative temperature coefficient thermistors, precise temperature sensors, in-rush current limiters, etc. Typically, structural properties of such materials re studied using different traditional method of structural characterizations. Our previous investigations have shown that the quantity of the additional defect-related phase and its distribution in bulk and on the surface of ceramics are influenced by temperature-time sintering regimes. Also, we used positron annihilation lifetime spectroscopy to study of free volumes defects in temperature-sensitive spinel ceramics. It is established that the amount of additional NiO phase in these ceramics extracted during sintering play a decisive role. The process of monolitization from the position of evolution of grain-pore structure was studied in these ceramics using positron annihilation lifetime spectroscopy within two-component fitting procedures. In addition, NiO phase results in transformation of free-volume defect-related places in the inner structure of ceramics. To study free-volume defects formed by NiO and nanopores in Cu0.1Ni0.8Co0.2Mn1.9O4 ceramics two and three-component fitting procedures and using positron-positronium trapping algorithm was used this work.

17:30 Extended free-volume defects in doped BaTiO3 ceramics **M.P.32** ☆

Authors : H. Klym (1), Kostiv (1), A.I. Popov (2)
Affiliations : (1) Lviv Polytechnic National University, Lviv,

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Ukraine (2) Institute of Solid State Physics, University of Latvia, Riga, Latvia

Resume : In this work microstructure and inner free-volume defects in undoped and Ca-doped BaTiO3 ceramics were studied using combined methods. Undoped BaTiO3 ceramics and doped with 5, 10 and 15 mol% of Ca were sintered at 1250 oC. The positron annihilation lifetime measurements were performed with an ORTEC spectrometer using 22Na source placed between two sandwiched ceramic samples. The obtained data were treated with LT computer program, the best results were obtained to two-component fitting procedures. In respect to SEM investigations, typical ceramic samples show grain-porous microstructure and assemblies of fractional grains. By accepting two-state positron trapping model, for polycrystalline ceramic materials the short lifetime of 1 0.15 ns is generally attributed to the free annihilation of positrons. This value also correlated with theoretically calculated free positron lifetime in BaTiO3. The obtained value is closed to BaTiO3 single crystal. The second lifetime 2 arises from annihilation of positrons at defect sites. The presently observed values of 2 0.32 ns which is believed to come from the annihilation of positrons at vacancy complexes formed between the oxygen vacancies and the metal ion vacancies. It is shown that 2 increases with rise of Ca amount in BaTiO3 ceramics from 5 to 10 mol% and decreases in samples with 15 mol% of Ca the intensity I2 decreases from 22 to 16 % and increases to 25 % in samples with 15 mol% of Ca. This indicates that doping of Ca results in increasing of the size of free-volume defects in ceramics and decreasing of their amount. So, process of agglomeration of defects is take place at posing of BaTiO3 ceramics By Ca in amount of 5 and 10 mol%, while future increasing the Ca content to 15 mol% leads to fragmentation of free-volume defects.

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17:30	Luminescence of cerium doped LYSO single crystals under VUV excitations		**M.P.33**	☆
17:30	Study of ion induced radiation effects in optical materials using synchrotron VUV techniques		**M.P.34**	☆
17:30	Nanostructurization of free-volume defects in GeS2-Ga2S3-CsCl chalcogenide glasses studied with positron-positronium trapping al		**M.P.35**	☆

Authors : H. Klym (1), A. Ingram (2), I. Karbovnyk (1,3), A.I. Popov (4)
Affiliations : (1) Lviv Polytechnic National University, Lviv, Ukraine (2) Opole University of Technology, Opole, Poland (3) Ivan Franko National University of Lviv, Lviv, Ukraine (4) Institute of Solid State Physics, University of Latvia, Riga, Latvia

Resume : Modern nanomaterials science are required new high-informative characterization instruments sensitive to free volumes in atomic and subatomic scales. One of such probes is positron annihilation lifetime (PAL) spectroscopy. This method can be applied to study atomistic imperfections in different solids. In application to semiconductors, this method allows identification of intrinsic free volumes owing to simple models considering competitive channels of positron trapping, where positrons trap (extended free-volume defects) and pick-off decaying of positron-electron (positronium Ps). But when dealing with nanomaterials possessing nanostructural

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inhomogeneities, the PAL method seems too ambiguous in view of numerous complications in the adequate interpretation of PAL spectra. In this work, we shall used modified positron-Ps trapping algorithm for analysis of PAL spectra of 80GeS2-20Ga2S3 chalcogenide glasses with different amount of CsCl, in particular, free-volume defect evolution processes caused by nanostructurization, where intrinsic inclusions can affect both positron- and Ps-trapping channels in the overall balance of annihilation events possible in a host matrix. Proposed approach allows description of nanostructurization in terms of substitutional positron-Ps trapping within the same host matrix (80GeS2-20Ga2S3), e.g. the process which occurs as a transformation of o-Ps-sites in a host matrix towards positron-trapping sites in a nanoparticle-modified material:(80GeS2-20Ga2S3)100-x-(CsCl)x, x = 0;5;10;15. By accepting a tightly connected nature of these PAL trapping sites, we can defined conditionally this approach as coupling x3-x2-decomposition algorithm to distinguish it from conventional x3-decomposition procedure, describing the PAL spectra in terms of admixed positron-Ps trapping. The quantitative characteristics of trapping-sites themselves as well as the occurring final interbalance in the PAL components are not too important. Within developed formalism grounded on coupling x3-x2-decomposition procedure, the physical characteristics of nanostructurized media can be presented to estimate interfacial void volumes responsible for positron trapping and characteristic bulk positron lifetimes in CsCl-affected inhomogeneous media.

17:30	Positron-positronium trapping defects near grain boundaries in the modified MgO-Al2O3 ceramics	**M.P.36**	☆

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Authors : H. Klym (1), A. Ingram (2), I. Hadzaman (3), A.I. Popov (4)
Affiliations : (1) Lviv Polytechnic National University, Lviv, Ukraine (2) Opole University of Technology, Opole, Poland (3) Ivan Franko Drohobych State Pedagogical University, Drohobych, Ukraine (4) Institute of Solid State Physics, University of Latvia, Riga, Latvia

Resume : The positron annihilation lifetime (PAL) spectroscopy method based on the fact that the unstable positron-electron system (positronium Ps) is repelled from ionic cores of atoms and tends to location in open pores. In the case of oxide water-immersed ceramics, two channels of PAL should be considered – the positron trapping and o-Ps decaying [1]. In general, these processes are independent ones. However, if trapping sites will appear in a vicinity of grain boundaries on defects neighboring with nanopores, they can become mutually interconnected resulting in a significant complication of the measured PAL spectra. In addition, adsorbed water influences on process near grain boundaries and in nanopores in the MgO-Al2O3 ceramics. To clarify this feature, we shall study the PAL characteristics of modified MgO-Al2O3 ceramics affected to water sorption treatment enhancing o-Ps decaying over positron trapping modes using positron-positronium trapping algorithm. To apply positron-positronium trapping algorithm it was shown that the chemical-adsorbed water vapor and defects modifies structural defects located at the grain boundaries in a vicinity of nanopores, this process being accompanied by void fragmentation during water adsorption and agglomeration during water desorption after drying.

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17:30	Structural and electrical study of PEDOT:PSS	**M.P.37**	

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nanocomposites before and after irradiation

Authors : Karbovnyk I.(1,2), I. Zhudenko (2,3) Chalyy D. (3), Klym H. (2)
Affiliations : (1) Ivan Franko National University of Lviv, Lviv, Ukraine (2) Lviv Polytechnic National University, Lviv, Ukraine (3) Lviv State University of Life Safety, Lviv, Ukraine

Resume : Nanocomposites formed by the addition of nanosized filling elements into dielectric (often polymer) matrix are known to have extraordinary mechanical, thermal and electrical properties [1]. Among such nanocomposites of significant interest are PEDOT:PSS polymer matrices reinforced with carbon nanotubes which show great potential for sensor and other applications [2]. This particular polymer is one of the most studied and a lot of works have contributed to better understanding of PEDOT/PSS tailorable properties. In this of work we experimentally analyze structural features and electrical behavior of PEDOT:PSS polymer layers with inclusions of high-purity single-walled (SWCNTs) or multi-walled carbon nanotubes (MWCNTs) before and after irradiation. All investigated samples show lowest impedance (highest conductivity) at room temperature and electrical conductivity decrease upon cooling. General trend is that Re(Z) slightly increases with frequency from 1 kHz to up to some threshold frequency and then drops rapidly. This threshold frequency for pure PEDOT:PSS and PEDOT:PSS/SWCNTs samples is about 100 kHz and is somewhat lower for composite layers with MWCNTs. Most notable temperature effect on the real part of the impedance of fabricated polymer/CNTs composite layers is that Re (Z) increases drastically starting from certain temperature, which is different for samples with different composition. For pure polymer this occurs already at 80…90 K and below 60 K Re

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(Z) is almost out of the measurable range. For layers reinforced with SWCNTs, increase of impedance is more gradual and even more so for MWCNTs-reinforced composites. In the latter case, reliable measurements can be performed even at temperatures as low as 40K. In samples with incorporated CNTs the conditions for residual water storage are potentially different due to structural changes introduced by specific nanofiller, so that time needed for complete water removal is different and the process is eventually finished at different temperature. This assumption is further supported by the fact that samples with MWCNTs show slower growth of real impedance with decreasing temperature and generally have higher conductivity at lowest measured temperatures. It has been demonstrated that composites reinforced with Boron, Nitrogen or Carbon elements in the form nanostructures dispersed in a matrix can provide radiation shielding for different range of energies and without the generation of harmful secondary particles. On the other hand, polymers reinforced with carbon nanotubes exhibit electrical response, strongly dependent on the absorbed dosage of radiation. The un-irradiated plate can be conductive or not, depending on the CNT doping level. If the level is above the threshold, the current is flowing across the plate, but that the conductive path can be destroyed by high enough dosage of radiation. Thus, one has a simple circuit breaker that will immediately signal about critical exposure, in case the protection layer can no longer stop the incoming rays. Experimental and theoretical studies of such structures will be discussed.

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17:30	Investigation of Radiation Damage Processes in Lithium Ceramics under High-Temperature Irradiation		**M.P.38**	☆
17:30	Investigation of the efficiency of shielding gamma and electron radiation by TeO2 - WO3 - Bi2O3 - MoO3 - SiO glasses.		**M.P.39**	☆
17:30	Ferromagnetic resonance in Fe/Nb/Fe/IrMn spin valves		**M.P.40**	☆
17:30	Study of Helium Swelling in SiC Ceramics		**M.P.41**	☆
17:30	Radiation-induced point defects and processes in ionic oxides – where we are standing now and what we understand better		**M.P.42**	☆
17:30	Thermostimulated luminescence measurements of neutron, electron irradiated and thermochemically-reduced Y3Al5O12 and Gd3Ga5O12		**M.P.43**	☆
17:30	Cathodoluminescence study of AlN nanotube/CsI scintillator and AlN nanotube/polymer composites.		**M.P.44**	☆

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17:30	Case analysis of self-trapped hole Vk center mobility in metal fluorides and fluoroperovskites		**M.P.45**	☆

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12:30	*Lunch*			
	Session 7 : NN			
14:30	The point defect segregation to grain boundaries in random Fe-Cr alloys: atomistic level modelling.		**M.7.1**	☆
14:45	First principles study of phonon splitting and anharmonicity in defected titanium disulfide (TiS2)		**M.7.2**	☆
15:00	Irradiation effects on the mechanical properties of polycrystalline BCC metals by machine learning based atomistic simulations		**M.7.3**	☆
15:30	*Coffee break*			
	Session 8 : NN			

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16:00	Heavy ion irradiation induced defects in emerging memory materials ? crystallinity, microstructure and electrical properties	**M.8.1**	☆
16:15	Experimental-theoretical analysis track effects in silicon nitride irradiated with swift heavy ions	**M.8.2**	☆
16:30	ABO3 perovskite as well as BaF2, CaF2 and SrF2 bulk and surface F-center first principles computations	**M.8.3**	☆
17:00	Calculated properties of the self-trapped exciton in diamond and related materials from DFT calculations	**M.8.4**	☆
17:15	Boron Nitride nanomaterials and their applications	**M.8.5**	☆

START AT	SUBJECT View All	NUM.	ADD
	Session 5 : NN		
09:00	Band Gap Engineering and Trap Depths of Intrinsic Point Defects in RAlO3 (R = Y, La, Gd, Yb, Lu) Perovskites	**M.5.1**	☆

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09:30	Implication of nanostructuring approaches in higher manganese silicides	**M.5.2**	☆
09:45	Magnetization of Magnetically Inhomogeneous Sr2FeMoO6-d Nanoparticles	**M.5.3**	☆
10:00	Defect-assisted ion transport in magneto-ionic functional oxides and nitrides probed by positrons	**M.5.4**	☆
10:15	Engineering of defect complexes in ZnO nanowires grown by chemical bath deposition using oxygen plasma treatment	**M.5.5**	☆
10:30	*Coffee break*		
	Session 6 : NN		
11:00	Impact of composition and crystal structure on luminescence and non-linear optical properties in the mid-infrared spectral range	**M.6.1**	☆
11:30	Designing Novel Strategy to Produce Active Nanohybrids in Sunlight for Purification of Water Based on Inorganic Nanolayers, Magn	**M.6.2**	☆

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11:45	NAMD simulations of Cl/TiO2(110)/water interface for photocatalytic seawater splitting		**M.6.3**	☆
12:00	Ab initio calculations of Cu-doped TiO2 thin films for antibacterial applications		**M.6.4**	☆
12:15	In-situ Raman spectroelectrochemical studies of carbon based materials using concentrated aqueous electrolyte solution		**M.6.5**	☆

Symposium organizers

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EUROPEAN MATERIALS RESEARCH SOCIETY

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