2015 EFRC PI MEETING – GRAPHIC AGENDA FOR MONDAY, OCTOBER 26, 2015

		A. Energy Storage	B. Solar Energy Conversion	C. Control at the Level of Electrons	D. Carbon Sequestration	E. Materials and Chemistry by Design	F. Catalysis
Room		*Thurgood Marshall E/N*	*Thurgood Marshall S/W*	*Lincoln 2*	*Lincoln 6*	*Lincoln 5*	*Lincoln 3/4*
Chair		*Craig Henderson*	*Christopher Fecko*	*Jim Rhyne*	*James Rustad*	*Tim Fitzsimmons*	*Mike Markowitz*
I-1	**1:10**	[**CEES**] Christopher Wolverton *Northwestern University* Why Not Both? High-Capacity Hybrid Li-ion/Li-oxygen Batteries	[**CASP**] Ashley Marshall** *NREL; University of Colorado* Understanding and Improving the Chemistry of Lead Chalcogenide Quantum Dots for PV	[**CES**] Ulrich Welp *ANL* Rapid Enhancement of the Critical Current of High-Performance Superconducting Wires	[**NCGC**] Ian C. Bourg *Princeton University* Microstructural Constraints on the Energy Technology Uses of Fine-Grained Sedimentary Rocks	[**IMASC**] E. Kaxiras *Harvard University* Multiscale Modeling of Surface Reactivity in Nanoporous Alloys	[**BETCy**] Michael Adams *University of Georgia* Electron Bifurcation in Managing Efficient Conversion of Electrochemical Potential into Chemical Bonds
I-2	**1:30**	[**NECCES**] Shyue Ping Ong *UC San Diego* An Integrated First Principles and Experimental Approach to Enabling Multi-Electron Lithium-Ion Battery Cathode	[**CE**] Marc Baldo *MIT* Exciton Fission and Fusion	[**EFree**] Ivan Naumov *Carnegie Institution of Washington* Transitions Between Insulating, Metallic and Superconducting States in Low-Z Materials	[**CFSES**] Anastasia G. Ilgen *SNL* Mancos Shale-Brine-CO_2 Interactions and the Long-term Stability of Shale Caprock	[**CME**] Simone Raugei *PNNL* Toward Design of Molecular Electrocatalysts by Computations	[**ICDC**] Omar K. Farha *Northwestern University; King Abdulaziz University* Single-site Nickel Hydrogenation Catalyst Supported on a Metal-Organic Framework Produced via ALD
I-3	**1:50**	[**NEES**] Chunsheng Wang *University of Maryland* Sulfides for Li-ion Batteries and Beyond	[**CASP**] Joseph M. Luther *NREL* Improving the Understanding of Quantum Dot Solar Cells by Modifying the Chemistry of PbS and PbSe Quantum Dots	[**CES**] Daniel Shoemaker *University of Illinois* Directed Synthesis and Fast Characterization of Correlated-Electron Materials for the Center for Emergent Superconductivity	[**NCGC**] Jonathan Ajo-Franklin *LBNL* Self-Sealing or Self-Enhancing? Observations of Fracture Evolution during CO_2 Induced Dissolution at *In-situ* …	[**CCEI**] Tyler R. Josephson** *University of Delaware* Revealing the Sugar Isomerization Mechanism on Homogeneous Sn-Silicate Catalysts	[**CME**] Molly O'Hagan *PNNL* Using Second-Coordination Sphere Strucutral Dynamics to Control H_2 Production Rates in $[Ni(PR_2NR'_2)_2]^{2+}$ Catalysts
I-4	**2:10**	[**m2M**] Alan C. West *Columbia University* Investigations of Mesoscale Transport Processes in Magnetite	[**CBES**] Emily Weiss *Northwestern University* Electron Ratchets	[**SHINES**] Chia-Ling Chien *Johns Hopkins University* Observation of p-Wave Superconductivity in Epitaxial Bi/Ni Bilayers	[**GSCO2**] Kristian Jessen *University of Southern California* Mass Transfer and Sorption in the Context of CO_2 Storage in Saline Formation	[**FIRST**] Peter T. Cummings *Vanderbilt University* Understanding and Predicting the Interfacial Structure and Dynamics in Capacitive Energy Systems Utilizing …	[**BETCy**] Anne Jones *Arizona State University* Defining Determinants of Catalytic Bias in Enzyme Catalyzed Proton-Coupled Electron Transfer Reactions
I-5	**2:30**	[**NEES**] Eleanor I. Gillette *University of Maryland* 3D Structure, Kinetics and Rate Performance in V_2O_5 Cathodes	[**CE**] William Tisdale *MIT* Exciton Dynamics in Hybrid 0D/2D Systems	[**CES**] Sean Vig** *University of Illinois* Characterization of the Low-Energy Bosonic Modes in $Bi_2Sr_2CaCu_2O_{8+x}$ with Incipient Charge Order	[**NCGC**] Lauren Beckingham# *LBNL* The Role of Advanced Reactive Surface Area Characterization in Improving Predictions of Mineral Reaction Rates …	[**UNCAGE-ME**] David A. Dixon *University of Alabama* Molecular and Dissociative Adsorption of Water on $(TiO_2)_n$ Clusters	[**CBES**] Samuel Stupp *Northwestern University* Center for Bio-Inspired Energy Science

2:50 – 3:20 PM Break

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		A. Energy Storage	B. Solar Energy Conversion	G. Synthesis of Functional Matter	H. Bioscience	E. Materials and Chemistry by Design	F. Catalysis
Room		*Thurgood Marshall E/N*	*Thurgood Marshall S/W*	*Lincoln 2*	*Lincoln 6*	*Lincoln 5*	*Lincoln 3/4*
Chair		*Jane Zhu*	*Christopher Fecko*	*Raul Miranda*	*Robert Stack*	*Mark Pederson*	*Viviane Schwartz*
II-1	**3:20**	[**FIRST**] Boris Dyatkin** *Drexel University* Probing Supercapacitor Carbon-Electrolyte Structure and Ion Dynamics with Neutrons	[**CASP**] Victor I. Klimov *LANL* Luminescent Solar Concentrators Using Engineered Quantum Dots	[**CNGMD**] David Ginley, Kristin Persson *NREL; UC Berkeley; LBNL* Approach to the Targeted Identification and Synthesis of Transition Metal Oxide Polymorphs	[**CLSF**] Daniel Cosgrove *Penn State University* Primary Cell Wall Structure in Plants: New Concepts, Some Remaining Enigmas	[**CCDM**] Jianwei Sun *Temple University* Testing and Applications of the SCAN MetaGGA, an Accurate and Efficient Nonempirical Density Functional	[**IMASC**] Branko Zugic# *Harvard University* Dynamic Evolution of Nanoporous Gold Catalysts During Activation and Selective Oxidation Reactions
II-2	**3:40**	[**m2M**] Esther S. Takeuchi *Stony Brook University* Probing the Limits of Electron and Ion Transport over Multiple Length Scales	[**LMI**] Harry A. Atwater *Caltech* Architecting Infrared Absorption and Emission – Control of both Amplitude and Phase	[**CBES**] Kyle Bishop *Penn State University* Shape Directed Dynamics of Active Colloids	[**C3Bio**] Nich Carpita *Purdue University* Structure and Synthesis of Cellulose	[**CES**] Lucas Wagner *University of Illinois* Searching for New Correlated Materials for Superconductivity	[**ICDC**] Connie C. Lu *University of Minnesota* Uniform Heterobimetallic Active Sites in Metal-Organic Frameworks
II-3	**4:00**	[**NECCES**] Aziz Abdellahi** *MIT* The Effect of Cation Disorder on the Li Intercalation Voltage of Transition Metal Oxides	[**S3TEC**] Marin Soljacic *MIT* Nanophotonics in Material-Systems of Large Sizes	[**MSA**] Peter C. Burns *University of Notre Dame* Aggregation and Solubility of Clusters of Actinides in Water	[**CLSF**] Venu Gopal Vandavasi# *ORNL* Structural Studies of Plant Cellulose Synthase Support 18 Synthases in the Cellulose Synthesis Complex	[**CNGMD**] William Tumas, Gerbrand Ceder *NREL; UC Berkeley; LBNL* Incorporating Metastabilty into Materials by Design	[**CGS**] Jeffrey A. Reimer *UC Berkeley* NMR Studies of Heterogeneity, Dynamics, and Phase Equilibria in MOFs
II-4	**4:20**	[**m2M**] Yimei Zhu *BNL* The Role of Structural Defects in $Ag_xMn_8O_{16-y}$ Hollandite Nanorods for Energy Storage	[**LMI**] Ralph G. Nuzzo *University of Illinois; Caltech* Optical Materials and Architectures for Ultrahigh-Efficiency Photovoltaics	[**EFree**] Stephen Juhl *Penn State University* Dispersion and High-Resolution Transmission Electron Microscopy of Carbon Nanothreads	[**C3Bio**] Bryon Donohoe *NREL* Altered Lignin Biosynthesis Tailors Plant Cell Wall Architecture for Efficient Catalytic Conversions to Fuels …	[**ICDC**] Laura Gagliardi, Joseph T. Hupp *University of Minnesota; Northwestern University* Inorganometallic Catalyst Design Center	[**IMASC**] Robert J. Madix *Harvard University* Probing Active Sites on npAuAg Alloy
II-5	**4:40**	[**FIRST**] Nina Balke *ORNL* Tracking Ions in Electrochemical Capacitors across Different Time and Length Scales	[**PARC**] Andrew Shreve *University of New Mexico* Energy Harvesting Using Random Assemblies of Chromophores	[**MSA**] Katlyn Turner** *Stanford University* Structural Evolution of Uranyl Peroxide Nano-Cage Fullerene: U60, at Elevated Pressures	[**CLSF**] Jochen Zimmer *University of Virginia* Mechanism of Cellulose Synthesis and Membrane Translocation	[**CGS**] Berend Smit *UC Berkeley* How to Quantify Similarity in Nanoporous Materials	[**ICDC**] Alex Martinson *ANL* Atomic Layer Deposition (ALD) in Metal Organic Frameworks (MOFs)

5:00 – 6:30 PM **Poster Session I (odd # posters), Exhibition Hall C**
6:30 – 7:30 PM **Science Trivia Night (students and postdocs only)**

		A. Energy Storage	B. Solar Energy Conversion	I. Separations	H. Bioscience	E. Materials and Chemistry by Design	F. Catalysis
Room		*Thurgood Marshall E/N*	*Thurgood Marshall S/W*	*Lincoln 2*	*Lincoln 6*	*Lincoln 5*	*Lincoln 3/4*
Chair		*Lane Wilson*	*Mark Spitler*	*Larry Rahn*	*Stephen Herbert*	*Jim Davenport*	*Michael Sennett*
III-1	**8:30**	[**NECCES**] Y. Shirley Meng *UC San Diego* Understanding the Layered Oxides for High-Voltage Intercalation in Alkaline Ion Batteries	[**ANSER**] Gary Brudvig *Yale University* Water-Oxidation Catalysts for Solar Fuel Production	[**MSA**] May Nyman *Oregon State University* Cluster-based Uranium Separation using Green Chemistry Principles	[**PARC**] Kaitlyn Faries** *Washington University in St. Louis* Expanding the Range of Light Absorbers for Bacterial Photosynthesis: YFP-Enhanced Charge Separation at the …	[**CCDM**] Liping Yu *Temple University* Designing Functional Two-Dimensional Materials by Bending	[**IMASC**] M. Flytzani-Stephanopoulos *Tufts University* Selective Methanol Dehydrogenation to Formaldehyde Across a Continuum of Structures: From Single Crystals to …
III-2	**8:50**	[**CEES**] Tim Fister *ANL* Interfacial Control of Oxide Conversion Reactions in Thin Film Battery Electrodes	[**FIRST**] Joel Rosenthal *University of Delaware* Insights into the Molecular Dynamics at the Cathode/Electrolyte Interface of Electrocatalyst Materials for CO_2 Reduction in …	[**CGS**] Jeffrey R. Long *UC Berkeley* Carbon Dioxide Capture in Diamine-Appended Metal-Organic Frameworks	[**BETCy**] Anne-Frances Miller *University of Kentucky* Flavins are Single-Molecule Switches that Couple Electron Transfer, Proton Transfer, Conformational Gating …	[**CE**] Jing Kong *MIT* Two Dimensional Transition Metal Dichalcogenide Materials through Chemical Vapor Deposition Synthesis	[**CCEI**] Michael Tsapatsis *University of Minnesota* Advances in Materials Synthesis for Biomass Conversion
III-3	**9:10**	[**NECCES**] Louis Piper *Binghamton University* Electrochemical Evolution of the Surface and Subsurface Properties of Layered Nickel-Rich Oxide Cathodes	[**ANSER**] Rebecca J. Lindquist** *Northwestern University* Incorporation of Perylene-3,4-dicarboximides into Photoanodes and Photocathodes for Solar Fuels	[**UNCAGE-ME**] Krista S. Walton *Georgia Tech* In situ IR Spectroscopic Investigation of Acid Gas Adsorption on MOF-Derived Ceria and Titania	[**PARC**] Volker Urban *ORNL* Neutron Scattering Studies of Photosynthetic Antenna Systems	[**CCDM**] Arun Bansil *Northeastern University* Spin-Polarization, Topological, Water-Splitting and Photo-Catalytic Properties of Ultrathin Films of Transition Metal …	[**ICDC**] Samuel O. Odoh# *University of Minnesota* Metal-Organic Framework Nodes as Nearly Ideal Supports for Molecular Catalysts: NU-1000- and UiO-66-Supported Iridium Complexes for Ethylene …
III-4	**9:30**	[**FIRST**] Michael Naguib *ORNL* 2D Transition Metal Carbides (MXenes) for Electrochemical Capacitors	[**CCDM**] Linyou Cao *North Carolina State University* Design of Multifunctional Two-Dimensional Materials: Toward Ideal Photocatalysts for Solar Water Splitting	[**CCEI**] J. Ilja Siepmann *University of Minnesota* Understanding Unique Diffusion Behavior in Hierarchical Zeolites	[**CBES**] Anna Balazs *University of Pittsburgh* Designing Self-regulating Microcapsules that Harness Chemical Energy to Undergo Bimimetic Collective Motion	[**CE**] Mircea Dinca *MIT* Two-Dimensional Charge Transport in Metal-Organic Frameworks	[**UNCAGE-ME**] Uma Tumuluri# *ORNL* Acid Gas Interaction with Oxide Nanoshapes with Well-defined Surface Facets
III-5	**9:50**	[**NEES**] Yue Qi *Michigan State University* Understanding the Science at Complex Interfaces for Nano-Structured Battery Design	[**UNC**] Gerald J. Meyer *University of North Carolina* Dye-Sensitized Water Oxidation in Photoelectrosynthesis Cells	[**Efree**] Max Murialdo** *Caltech* Anomalous Surface Thermodynamics of Gas Adsorption on Zeolite-Templated Carbon	[**PARC**] Aparna Nagarajan *Washington University* Phycobilisome Degradation in a Fast Growing Cyanobacterium	[**SHINES**] Nathaniel Gabor *UC Riverside* Spatio-Temporal Imaging of Spin, Valley, and Thermal Energy in Two-Dimensional Materials	[**IMASC**] Cynthia Friend *Harvard University* Informing Catalyst Design through Fundamental Studies

10:10 – 10:40AM Break

		J. Mesoscale Science	B. Solar Energy Conversion	C. Control at the Level of Electrons	D. Carbon Sequestration	E. Materials and Chemistry by Design	F. Catalysis
Room		*Thurgood Marshall E/N*	*Thurgood Marshall S/W*	*Lincoln 2*	*Lincoln 6*	*Lincoln 5*	*Lincoln 3/4*
Chair		*Philip Wilk*	*Refik Kortan*	*Michael Pechan*	*P. Thiyagarajan*	*John Vetrano*	*Wade Sisk*
IV-1	**10:40**	[**EDDE**] Yanwen Zhang *ORNL* Influence of Chemical Disorder on Energy Dissipation and Defect Evolution in Advanced Alloys - Progress toward Structural Materials by …	[**ANSER**] Mercouri Kanatzidis *Northwestern University* Lead Free Inorganic-Organic Hybrid Perovskites: Chemistry and Solar Cells	[**MSA**] Albert Migliori *LANL* Precision Plutonium Thermodynamics-Equilibria, Kinetics, and Complications	[**NCGC**] Andrew G. Stack *ORNL* Pore-Size Dependent Mineral Reactions in Porous Media	[**CNGMD**] Lauren Garten[#] *NREL* Predicting and Controlling Polymorphism in Transition Metal Oxides	[**CCEI**] Eyas Mahmoud *University of Delaware* Diels-Alder and Dehydration Reactions of Biomass-Derived Furan and Acrylic Acid for the Synthesis of Benzoic Acid
IV-2	**11:00**	[**CLSF**] Candace Haigler *North Carolina State University* Leveraging Empirical and Computationally Modeled Structures to Explore Plant Cellulose Synthase Protein Function	[**CNGMD**] Riley Brandt, Vladan Stevanovic *MIT; Colorado School of Mines* Perovskite Inspired Search for New PV Materials	[**S3TEC**] Bolin Liao *MIT* Understanding Electron Transport in Thermoelectrics from First-principles	[**GSCO2**] Kenneth T. Christensen *University of Notre Dame; Kyushu University* Pore-Scale Phenomena Affecting Transport and Fate of Supercritical CO_2 in Geological Reservoirs: Flow Dynamics, …	[**EDDE**] Ian M. Robertson *University of Wisconsin* Damage Production in Single-Phase Concentrated Solid Solution Alloys	[**C3Bio**] Maureen McCann *Purdue University* Delivering Fit-for-Purpose Biofuels
IV-3	**11:20**	[**MSA**] Maik Lang *University of Tennessee* Advanced Characterization Techniques for Actinide Materials	[**ANSER**] Tobin Marks *Northwestern University* Interface Science of Soft Matter Solar Cells	[**SHINES**] Javier Garay *UC Riverside* Producing Nanocrystalline Magnetic Insulators for Spin and Thermal Conductivity Studies	[**CFSES**] Tip Meckel *UT Austin* Constraining the Influence of Meso-scale Heterogeneity on CO_2 Saturation Resulting from Buoyant Flow using …	[**CNGMD**] Janet Tate, Aaron Holder *Oregon State University; NREL* Metastable Heterostructural Alloys	[**CCEI**] Alexander V. Mironenko *University of Delaware* Metal/Lewis Bifunctional Catalysts for Low Temperature Upgrade of Biomass
IV-4	**11:40**	[**CLSF**] Christopher Lee *Penn State University* Probing the Architecture of Plant Cell Wall In-between the Nanoscopic and Macroscopic Length Scales with Sum-Frequency-Generation (SFG) Vibration Spectroscopy	[**EFree**] Timothy A. Strobel *Carnegie Institution of Washington* Materials for Solar Energy Conversion Using Extreme Conditions: An Overview	[**CES**] J.C. Seamus Davis *BNL* Interplay of d-Symmetry Cooper Pairs and d-Symmetry Density Waves within the Cuprate Pseudogap Phase	[**UNCAGE-ME**] Christopher W. Jones *Georgia Tech* Neutron Scattering Links CO_2 Adsorption Performance to Polymer Morphology in Silica/PEI Composite Adsorbents	[**EDDE**] Laurent K Béland *ORNL* Modeling Primary Damage Production and Evolution in Concentrated NiFe	[**C3Bio**] Mahdi Abu-Omar *Purdue University* Selective Conversion of Lignin First in Total Utilization of Biomass to Make Fuels and Chemicals

12:00 – 1:30 PM Lunch

2015 EFRC PI MEETING – GRAPHIC AGENDA FOR TUESDAY, OCTOBER 27, 2015

		A. Energy Storage	B. Solar Energy Conversion	G. Synthesis of Functional Matter	D. Carbon Sequestration	E. Materials and Chemistry by Design	F. Catalysis
Room		*Thurgood Marshall E/N*	*Thurgood Marshall S/W*	*Lincoln 2*	*Lincoln 6*	*Lincoln 5*	*Lincoln 3/4*
Chair		*Craig Henderson*	*George Maracas*	*Bonnie Gersten*	*P. Thiyagarajan*	*Matthias Graf*	*Robert Stack*
V-1	**1:30**	[**CEES**] Mark Hersam *Northwestern University* Suppressing Manganese Dissolution from Lithium Manganese Oxide Cathodes with Single-Layer Graphene	[**CASP**] Alexander L. Efros *George Mason; NRL* Modeling of the Electronic Structure of Semi-conductor Nanocrystals, and Carrier Transport in Nanocrystal Arrays	[**CGS**] Lorenzo Maserati[#] *LBNL* Ultrafast Synthesis Metal-Organic Frameworks Critical for Energy-Efficient CO_2 Capture	[**CFSES**] Thomas Dewers *SNL* Geomechanics and Research Challenges for Geologic Carbon Storage	[**S3TEC**] Gang Chen *MIT* Probing and Understanding Thermal Transport and Energy Conversion In Nanostructures	[**BETCy**] Lance Seefeldt *Utah State University* Unraveling Nitrogenase Energy Conversion and Electron Transfer
V-2	**1:50**	[**NEES**] A. Alec Talin *SNL* The Challenge of 3D All Solid State Li-ion Battery	[**UNC**] Thomas J. Meyer *University of North Carolina* Systems and Assemblies for Applications in Dye-Sensitized Photo-electrosynthesis Cells	[**LMI**] Jennifer A. Lewis *Harvard University* Printing Functional Materials	[**NCGC**] Carl I. Steefel *LBNL* Pore-Scale and Continuum Modeling of Fracture Evolution and Mineral Trapping during CO_2 Sequestration	[**EDDE**] G. Malcolm Stocks *ORNL* Extreme Chemical Complexity: A Route to the Control of Energy Dissipation and Defect Evolution in Structural Materials for Intense …	[**UNCAGE-ME**] Israel E. Wachs *Lehigh University* Defects Matter: Co-precipitated and Impregnated Supported WO_3/TiO_2 and V_2O_5-WO_3/TiO_2 Catalysts for ...
V-3	**2:10**	[**m2M**] Kenneth J. Takeuchi *Stony Brook University* Structure-Function Relationships of Electroactive Materials Modulated by Synthetic …	[**CASP**] Matt Law *UC Irvine* Charge Transport in Mesoscale Assemblies of Quantum Dots	[**CGS**] Michael Tsapatsis *University of Minnesota* Advances in 2-Dimensional Porous Layers for Gas Separation Membranes	[**GSCO2**] Michael Jordan *SINTEF Petroleum Research* Improved Quantification of Reservoir Parameters from Seismic Data	[**S3TEC**] David Broido *Boston College* Phonon Thermal Transport in Thermoelectric Materials from First Principles	[**CME**] Michael T. Mock *PNNL* Exploring the Role of Pendant Amines in Metal Complexes for N_2 Reduction and NH_3 Oxidation
V-4	**2:30**	[**CEES**] Nancy R. Sottos *University of Illinois* Electrochemical Stiffness in Lithium-ion Batteries – A New Concept for Understanding Electrode Response	[**UNC**] John M. Papanikolas *University of North Carolina* Ultrafast Dynamics in Molecular Assemblies for Solar Energy Conversion	[**EFree**] Yiqun Liu *Lehigh University* Synthesis of Periodic Mesoporous Silica With Crystalline Pore Walls	[**CFSES**] Marc A. Hesse *UT Austin* Constraints on Long-term Safety of Geological CO_2 Storage from Natural Analogues	[**LMI**] Austin J. Minnich *Caltech* Spectrally Selective Semiconductor Absorbers for Solar Thermal Energy Conversion	[**ANSER**] Alex Martinson *ANL* Atomic Layer Epitaxy of Fe_2O_3 for New Frontiers in Photo-Assisted Water Oxidation
V-5	**2:50**	[**NECCES**] Karena Chapman *ANL* Advancing Operando Tools to Probe Multiscale Complexity in Chemical Energy Storage	[**PARC**] Jonathan Lindsey *North Carolina State University* Biohybrid Light-Harvesting Architectures - Blending Chemistry and Biology	[**UNC**] James F. Cahoon *University of North Carolina* Designing Photocathode Materials For Dye-Sensitized Photo-electrosynthesis Cells	[**GSCO2**] Volker Oye *NORSAR* Induced Seismicity Due to Low Pressure-Gradient Fluid Injections: Linking Laboratory-Scales with Field-Scale Observations	[**SHINES**] Jing Shi *UC Riverside* Topological Spin Seebeck Effect in Topological Insulator/Yttrium Iron Garnet Heterostructures	[**CME**] James M. Mayer *Yale University* Molecular Catalysts for the Oxygen Reduction Reaction (ORR)

3:10 – 5:00 Poster Session II (even # posters), Exhibition Hall C; 4:00 Announce winners of the *Graduate Student and Postdoctoral Researcher Competition*