

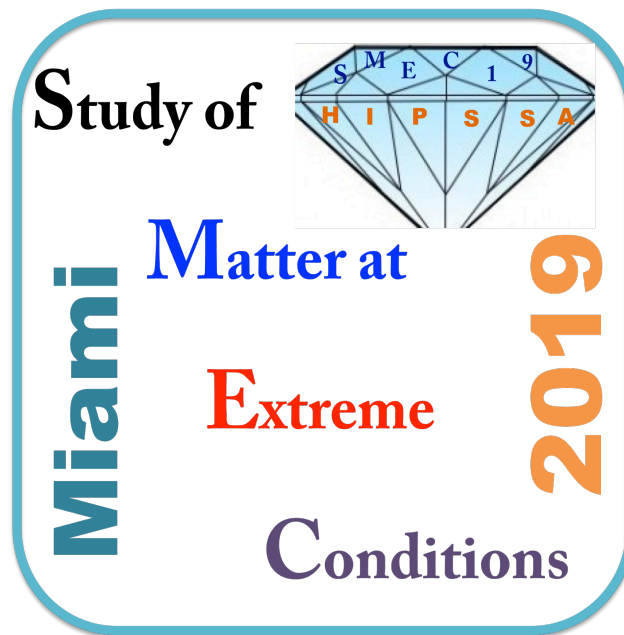
International Meeting on

**Study of matter at extreme conditions (SMEC2019)**

**March 30 - April 06, 2019**

**Miami - East Caribbean - Miami**

## **SCIENTIFIC PROGRAM**



International meeting on

**Study of Matter at Extreme Conditions**

**March 30 - April 06, 2019**

**Conference Center, Celebrity Equinox**

## Celebrity Equinox, March 30 – April 6, 2019

### Cruise Itinerary

Date	Port Location	Arrive	Depart
30 MAR	MIAMI, FLORIDA		3:30 PM
31 MAR	AT SEA		
01 APR	SAN JUAN, PUERTO RICO	3:30 PM	11:00 PM
02 APR	CHARLOTTE AMALIE, ST. THOMAS	8:00 AM	5:00 PM
03 APR	PUNTA CANA, DOMINICAN REP	7:00 AM	5:00 PM
04 APR	AT SEA		
05 APR	NASSAU, BAHAMAS	9:00 AM	6:00 PM
06 APR	MIAMI, FLORIDA	7:00 AM	



## PROGRAM AT A GLANCE

Saturday March 30, 2019	
15:00-18:30	<b>Registration</b> – conference center, <i>Celebrity Equinox</i>
18:30-20:00	<b>SMEC Reception &amp; Welcome Party</b> – venue to be communicated

Sunday March 31, 2019		
8:30-10:30	<b>Opening &amp; Plenary Session</b>	
10:30-11:00	<b>Coffee Break</b>	
11:00-12:30	Symposium 6, <i>Recent developments in topological and correlated materials.</i> Symposium 7, <i>Emerging layered superconductors and related materials.</i>	Symposium 2, <i>Multifunctional metal hydrides for energy storage.</i> Symposium 3, <i>Materials for energy applications.</i>
12:30-14:00	<b>Lunch Break</b>	
14:00-16:00	Symposium 6, <i>Recent developments in topological and correlated materials.</i> Symposium 7, <i>Emerging layered superconductors and related materials.</i>	Symposium 2, <i>Multifunctional metal hydrides for energy storage.</i> Symposium 3, <i>Materials for energy applications.</i>
16:00-16:30	<b>Coffee Break</b>	
16:30-18:30	Symposium 6, <i>Recent developments in topological and correlated materials.</i> Symposium 7, <i>Emerging layered superconductors and related materials.</i>	Symposium 2, <i>Multifunctional metal hydrides for energy storage.</i> Symposium 3, <i>Materials for energy applications.</i>

Monday April 01, 2019		
8:30-10:30	Symposium 6, <i>Recent developments in topological and correlated materials.</i> Symposium 7, <i>Emerging layered superconductors and related materials.</i>	Symposium 2, <i>Multifunctional metal hydrides for energy storage.</i> Symposium 3, <i>Materials for energy applications.</i>
10:30-11:00	<b>Coffee Break</b>	
11:00-12:30	Symposium 6, <i>Recent developments in topological and correlated materials.</i> Symposium 7, <i>Emerging layered superconductors and related materials.</i>	Symposium 2, <i>Multifunctional metal hydrides for energy storage.</i> Symposium 3, <i>Materials for energy applications.</i>
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Tuesday April 02, 2019	
08:30-10:00	Symposium 6, <i>Recent developments in topological and correlated materials.</i> Symposium 3, <i>Materials for energy applications.</i>
16:30-18:30	Symposium 12, <i>50 Years of high pressure superconductivity research.</i> Symposium 7, <i>Emerging layered superconductors and related materials.</i>

Wednesday April 03, 2019	
08:30-09:30	<i>Graduate Students Session – I</i>
16:30-18:30	<i>Graduate Students Session – II &amp; Posters</i>

Thursday April 04, 2019	
08:30-10:30	Symposium 5, <i>Unconventional superconductivity in Fe-based materials under extreme conditions.</i>
10:30-11:00	<b>Coffee Break</b>
11:00-12:30	Symposium 5, <i>Unconventional superconductivity in Fe-based materials under extreme conditions.</i>
	Symposium 9, <i>High pressure planetary and earth sciences.</i>
12:30-14:00	<b>Lunch Break</b>
14:00-16:00	Symposium 5, <i>Unconventional superconductivity in Fe-based materials under extreme conditions.</i>
	Symposium 9, <i>High pressure planetary and earth sciences.</i> Symposium 10, <i>Two-dimensional materials: graphene and beyond.</i>
16:00-16:30	<b>Coffee Break</b>
16:30-18:30	Symposium 5, <i>Unconventional superconductivity in Fe-based materials under extreme conditions.</i>
	Symposium 6, <i>Recent developments in topological and correlated materials.</i> Symposium 4, <i>Quantum emergent matters: materials &amp; phenomena driven by extreme conditions.</i>

Friday April 05, 2019	
08:30-10:30	Symposium 7, <i>Emerging layered superconductors and related materials.</i>
17:00-19:00	Symposium 10, <i>Two-dimensional materials: graphene and beyond.</i>

18:00-19:00	<b>Closing &amp; Concluding Remarks</b>
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# DETAILED SCIENTIFIC PROGRAM

Sunday March 31, 2019

S-1

Room 1	
<b>Opening Plenary Session</b>	
<b>Chairs: S. Saxena, R. Hennig</b>	
08:30-09:30	H. K. Mao, <i>Recent advances in high-pressure physics, materials, and geoscience.</i>
09:30-10:30	A. Bansil, <i>Raising the bar toward a first-principles description of stronger correlations: Novel superconductors to topological materials.</i>

10:30-11:00      **Coffee Break**

S-2A

S-2B

Room 1		Room 2
<b>Topological &amp; Correlated Materials-1</b>		<b>Metal Hydrides &amp; Energy Materials-1</b>
<b>Chairs: A. Bansil, X. X. Xi</b>		<b>Chairs: H.-W. Li, J. Chen</b>
11:00-11:30	K. Tanigaki, <i>Single crystal thin films of three-dimensional topological insulators via non-catalytic vapor phase epitaxial crystal growth.</i>	C. J. Webb, <i>The use of oxides to kinetically enhance the sorption properties of MgH<sub>2</sub> at high pressure.</i>
11:30-12:00	T. H. Choudhury, <i>Controlling epitaxial growth of transition metal dichalcogenides by gas source CVD.</i>	C. Jensen, <i>Reversible Hydrogenation of Magnesium Boride and Magnesium Boranes to Magnesium Borohydride.</i>
12:00-12:30	Z. Mao, <i>Layered magnetic topological semimetals and their unusual interlayer quantum transport.</i>	T. R. Jensen, <i>Hydrogen storage and battery materials - new types of materials.</i>

12:30-14:00      **Lunch Break**

S-3A		S-3B	
	Room 1	Room 2	
	<b>Topological &amp; Correlated Materials-2</b>	<b>Metal Hydrides &amp; Energy Materials-2</b>	
	<b>Chairs: K. Tanigaki, B. Barbiellini</b>	<b>Chairs: T.R. Jensen, C.J. Webb</b>	
14:00–14:30	Qi Li, <i>Topological Surface States and Inducing Superconductivity in Bi<sub>2</sub>Te<sub>3</sub> Nanotubes.</i>	V. Yartys, <i>High pressure metal hydrides for hydrogen based energy storage: structure-properties relationship.</i>	
14:30-15:00	L. Balicas, <i>Topological Semimetals from a High Magnetic Fields Perspective.</i>	K. T. Møller, <i>Molten metal closo-hydridoborates.</i>	
15:00-15:30	S. Y. Matsushita, <i>Quantum hall effect and thermoelectric properties of surface Dirac states in Sn-Bi<sub>1.1</sub>Sb<sub>0.9</sub>Te<sub>2</sub>S crystal.</i>	Y. Filinchuk, <i>Non-equilibrium Kr adsorption in nanoporous <math>\gamma</math>-Mg(BH<sub>4</sub>)<sub>2</sub> by in situ synchrotron powder diffraction.</i>	
15:30-16:00	I. Dasgupta, <i>Realization of Spin-Orbital Liquid State in Iridates.</i>	C. Zlolea, <i>Multi-principal-element alloys as new materials for hydrogen absorption.</i>	

16:00-16:30	<b>Coffee Break</b>
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S-4A		S-4B	
	Room 1	Room 2	
	<b>Topological &amp; Correlated Materials-3</b>	<b>Metal Hydrides &amp; Energy Materials-3</b>	
	<b>Chairs: J. Sun, J.F. He</b>	<b>Chairs: Y. Filinchuk, D. Matsumara</b>	
16:30-17:00	Y. Ding, <i>Spin-Orbit Assisted Correlated Materials at High Pressure: Novel Phases and Phenomena.</i>	M. Polanski, <i>H<sub>2</sub> Nautic - a hydrogen storage vessel for small touristic boats.</i>	
17:00-17:30	T. Schmitt, <i>Evolution of the spin, orbital and charge excitations upon tuning the local lattice environment of Sr<sub>2</sub>IrO<sub>4</sub>.</i>	M. Heere, <i>Complex metal hydrides investigated by fast neutron powder diffraction.</i>	
17:30-18:00	W. S. Kyung, <i>Electric field driven octahedral rotation in Sr<sub>2</sub>RuO<sub>4</sub> and its implication.</i>	Y. Song, <i>Structural Stability of and Enhanced CO<sub>2</sub> Storage in Metal-Organic Frameworks under High Pressures Probed by Vibrational Spectroscopies and X-ray Diffraction.</i>	
18:00-18:30	O. Eriksson, <i>DMFT coupled to DFT: Case of some complex oxides.</i>		

**Monday April 01, 2019**

S-5A		S-5B	
	Room 1		Room 2
	<b>Topological &amp; Correlated Materials-4</b>		<b>Metal Hydrides &amp; Energy Materials-4</b>
	<b>Chairs: A. Bansil, T. Schmitt</b>		<b>Chairs: Y. Filinchuk, R. Ahuja</b>
08:30-09:00	D. Dessau, <i>High temperature and possible topological superconductivity.</i>		C. E. Buckley, <i>Thermal Battery Development for Concentrated Solar Power Systems.</i>
09:00-09:30	M. Shi, <i>ARPES on topological quantum materials: from topological Kondo insulator to Weyl semimetal.</i>		L. Stievenano, <i>The sodiation-desodiation mechanism of Sb-based electrode materials revealed by operando spectroscopy assisted by chemometric data analysis.</i>
09:30-10:00	J. -F. He, <i>Angle-resolved photoemission studies on strongly correlated materials.</i>		M. Heere, <i>Neutron diffraction for energy storage and conversion in metal hydrides.</i>
10:00-10:30	N. L. Saini, <i>Electronic phase separation in BiS<sub>2</sub>-based systems.</i>		H. Miyaoka, <i>Study on catalytic activation for Mg hydrogen storage.</i>

10:30-11:00	<b>Coffee Break</b>
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S-6A		S-6B	
	Room 1		Room 2
	<b>Emerging Superconductors</b>		<b>Metal Hydrides &amp; Energy Materials-5</b>
	<b>Chairs: S. Feng, M. Shi</b>		<b>Chairs: C.E. Buckley, H. Miyaoka</b>
11:00-11:30	D. Louca, <i>Nanoscale Atomic Distortions in the BiS<sub>2</sub> Superconductors: Ferrodistoritive Sulfur Modes.</i>		H. Saitoh, <i>High-pressure and high-temperature synthesis of novel hydrides.</i>
11:30-12:00	K. Kudo, <i>Superconductivity in Pt-based pnictides with ordered honeycomb networks.</i>		H. -W. Li, <i>Solvent-free Facile Synthesis of Metal Boron Hydrides for Superionic Conductivity.</i>
12:00-12:30	Y. Goto, <i>SnPn-based layered superconductors.</i>		K. T. Møller, <i>Thermochemical Energy Storage Utilising Metal Carbonates.</i>

12:30-14:00	<b>Lunch Break</b>
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S-7A

S-7B

	Room 1	Room 2
	<b>Topological &amp; Correlated Materials-5</b>	<b>Metal Hydrides &amp; Energy Materials-6</b>
	<b>Chairs: Y. Ding, D. Dessau</b>	<b>Chairs: T.R. Jensen, V. Yartys</b>
14:00-14:30	S. Zhang, <i>Dark and half excitonic insulators.</i>	C. Pistidda, <i>A Hydride Composite Featuring Mutual Destabilisation and Reversible Boron Exchange: Ca(BH<sub>4</sub>)<sub>2</sub>-Mg<sub>2</sub>NiH<sub>4</sub>.</i>
14:30-15:00	M. R. Vega, <i>Higher-order Floquet topological phases with corner and bulk bound states.</i>	D. Matsumura, <i>X-ray absorption spectroscopy for reaction of metal hydrides.</i>
15:00-15:30	T. S. Dasgupta, <i>Heterostructures of 3d-5d Double Perovskites: Potential Candidates for Confined Half-metallicity &amp; High-T Quantum Anomalous Hall States.</i>	M. Polanski, <i>What hydride can steal from stainless steel ? About the Mg<sub>2</sub>FeH<sub>6</sub> formation from magnesium hydride and austenitic steel.</i>
15:30-16:00	X. Wan, <i>Towards ideal topological materials: Comprehensive database searches using symmetry indicators.</i>	



Tuesday Aril 02, 2019

S-8

Room 1	
Correlated Oxides & Energy Materials	
Chairs: I. Dasgupta, N.L. Saini	
08:30-09:00	X. X. Xi, <i>Nature of the metal-insulator transition in few-unit-cell-thick LaNiO<sub>3</sub> films.</i>
09:00-09:30	B. Barbiellini, <i>Identification of ferrimagnetic orbitals preventing Jahn-Teller distortions in Li<sub>x</sub>Mn<sub>2</sub>O<sub>4</sub> cathodes.</i>
09:30-10:00	S. H. Lee, <i>New Materials for Next Generation Printable Solar Cells.</i>

16:00-16:30

Coffee Break

S-9

Room 1	
High Pressure Superconductivity	
Chairs: R. Hennig, A. Bansil	
16:30-17:30	W. Pickett, <i>How Compressed Hydride Superconductors Produce Room Temperature Superconductivity.</i>
17:30-18:00	E. Zurek, <i>Computational Discovery of Novel Superconducting Hydride Phases Under Pressure.</i>
18:00-18:30	T. Shibauchi, <i>High-T<sub>c</sub> superconducting phases of FeSe-based materials at high pressure.</i>

Wednesday April 03, 2019

**S-10**

	<b>Room 1</b>
	<b>Graduate Students Session-I</b>
	<b>Chairs: M. Polanski, C. E. Buckley</b>
08:30-08:45	M. Jørgensen, <i>Weakly coordinating anions in solid state electrolytes.</i>
08:45-09:00	J. B. Grinderslev, <i>Extreme Hydrogen Densities in Ammonium Metal Borohydrides.</i>
09:00-09:15	M. Pęska, <i>Magnesium – Lithium alloys as hydrogen storage materials.</i>
09:15-09:30	J. Vodeb, <i>Correlated Configurational States and a Quantum Charge Liquid in Layered Metallic Dichalcogenides.</i>

16:00-16:30

**Coffee Break**

**S-11**

	<b>Room 1</b>
	<b>Graduate Students Session-II</b>
	<b>Chairs: N. L. Saini, K. Kudo</b>
16:30-16:45	S. R. Xie, <i>Machine learning of Potential-Energy Landscapes in Two-dimensional Group-III Oxides.</i>
16:45-17:00	P. Nautiyal, <i>Graphene Foam for Engineering Ultra-Stiff, Tough and Impact-Resistant Structural Composites.</i>
17:00-17:15	J. T. Paul, <i>Materials Informatics Search for Strongly Correlated 1D Materials.</i>
17:15-18:30	Poster Presentations (Pugliese, Stramaglia, Shinzato, Karczewski)
17:45-18:30	

**Thursday April 04, 2019**

**S-12**

<b>Room 1</b>	
<b>Iron-based Superconductors - 1</b>	
<b>Chairs: C. Meingast, B. Buechner</b>	
08:30-09:00	P. Hirschfeld, <i>Pairing mechanism in iron-based superconductors: variations on the s+/- theme.</i>
09:00-09:30	Y. Li, <i>Spin-orbit coupling and "preferred" magnetic excitations in iron-based superconductors.</i>
09:30-10:00	R. Hackl, <i>Microscopic origin of Cooper pairing in <math>Ba_{1-x}K_xFe_2As_2</math> and <math>CaKFe_4As_4</math>.</i>
10:00-10:30	F. Hardy, <i>Nodal Superconductivity in FeSe single crystals from heat capacity.</i>

**10:30-11:00 Coffee Break**

**S-13A**

**S-13B**

<b>Room 1</b>		<b>Room 2</b>
<b>Iron-based Superconductors - 2</b>		<b>High Pressure Earth &amp; Planetary Sci.</b>
<b>Chairs: P. Hirschfeld, F. Hardy</b>		<b>Chairs: J. Chen, S. Saxena</b>
11:00-11:30	B. M. Andersen, <i>Multi-orbital effects and the role of spin-orbit coupling in iron-based superconductors.</i>	Han Hsu, <i>Iron spin crossover in the Earth and planetary interiors: A perspective from computational materials physics.</i>
11:30-12:00	B. Buechner, <i>Orbitals and Nematicity in La-1111 Single Crystals.</i>	M. Hou, <i>Temperature-induced amorphization in <math>CaCO_3</math> at high pressure: implication for recycled <math>CaCO_3</math> in subduction zones.</i>
12:00-12:15	A. P. Dioguardi, <i><math>^{75}As</math> NMR under uniaxial pressure in <math>BaFe_2As</math>.</i>	W. L. Mao, <i>Hydrogen-bearing iron peroxide in Earth's lowermost mantle.</i>
12:15-12:30	M. He, <i>Ubiquitous dichotomy between the in-plane uniform magnetic susceptibility and resistivity anisotropies in iron-based superconductors.</i>	W. L. Mao, <i>Hydrogen-bearing iron peroxide in Earth's lowermost mantle.</i>

**12:30-14:00 Lunch Break**

S-14A		S-14B	
	Room 1		Room 2
	<b>Iron-based Superconductors - 3</b>		<b>High Pressure &amp; 2D Materials</b>
	<b>Chairs: B.M Andersen, R. Hackl</b>		<b>Chairs: W.L. Mao, A. L. da Rosa</b>
14:00-14:30	T. Shibauchi, <i>Novel electronic nematicity in (Ba,Rb)Fe<sub>2</sub>As<sub>2</sub>.</i>		Jin Liu, <i>Mantle-Slab Interactions and Mantle Heterogeneities.</i>
14:30-15:00	M. S. Ikeda, <i>Feeling strain – Thermal and Resistive response in iron pnictides.</i>		Jiuhua. Chen, <i>Kinetics of dehydrogenation of FeOOH at Earth’s lower mental conditions.</i>
15:00-15:30	M. Christensen, <i>Intertwined spin-orbit coupled orders in the iron-based superconductors.</i>		A. Agarwal, <i>Graphene Foam-Based Multifunctional Polymer Composites for Self-Healing, De-icing and Strain-sensing Applications.</i>
15:30-15:45	C. Meingast, <i>Intertwined and vestigial electronic phases in hole-dopes Sr<sub>1-x</sub>Na<sub>x</sub>Fe<sub>2</sub>As<sub>2</sub>.</i>		O. Kurakevych, <i>Accomplishing a suite of magnesium carbides by HPHT synthesis.</i>
15:45-16:00	C. Meingast, <i>Intertwined and vestigial electronic phases in hole-dopes Sr<sub>1-x</sub>Na<sub>x</sub>Fe<sub>2</sub>As<sub>2</sub>.</i>		A. Soldatov, <i>Nanostructured graphene: When disorder makes things better?</i>

16:00-16:30	<b>Coffee Break</b>
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S-15A		S-15B	
	Room 1		Room 2
	<b>Iron-based Superconductors - 4</b>		<b>Topological &amp; Quantum Materials</b>
	<b>Chairs: Y. Li, T. Shibauchi</b>		<b>Chairs: A, Bansil, R. Hennig</b>
16:30-17:00	V. Taufour, <i>Pressure dependence of the superconducting upper critical field in KFe<sub>2</sub>As<sub>2</sub> and related materials.</i>		P. Vashishta, <i>Reactive molecular dynamics simulations and machine learning.</i>
17:00-17:30	G. Garbarino, <i>Pressure temperature phase diagram of iron based superconductors.</i>		E. Zurek, <i>Predicting Superhard Materials via a Machine Learning Informed Evolutionary Structure Search.</i>
17:30-18:00	V. Svitlyk, <i>Structure-property correlations in FeSe-based superconducting materials,</i>		J. Sun, <i>The SCAN density functional and its surprising performance in complex materials.</i>
18:00-18:15	N. L. Saini, <i>Local structure and superconductivity in iron-based superconductors.</i>		A. Nevidomskyy, <i>Emergent Spin Vortex Crystals in Frustrated Quantum Magnets.</i>
18:15-18:30			A. Nevidomskyy, <i>Emergent Spin Vortex Crystals in Frustrated Quantum Magnets.</i>

18:45-20:15	<b>Get Together Party</b> – venue to be communicated
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Friday April 05, 2019

S-16

<b>Room 1</b>	
<b>Correlated Materials &amp; Superconductivity</b>	
<b>Chairs: D. Louca, E. Zurek</b>	
08:30-09:00	K. Tanigaki, <i>Electron-phonon and electron-electron interactions in electron doped aromatic carbon materials viewed from electrical transport.</i>
09:00-09:30	S. Tsuchiya, <i>Development of optical pump probe spectroscopy under uniaxial pressure: Application to strongly correlated superconductors.</i>
09:30-10:00	K. Park, <i>Projected BCS theory for the unification of antiferromagnetism and strongly correlated superconductivity.</i>
10:00-10:30	S. Feng, <i>Autocorrelation of quasiparticle spectral intensities and its connection with quasiparticle scattering interference in cuprate superconductors.</i>

16:30-17:00

Coffee Break

S-17

<b>Room 1</b>	
<b>2D Materials &amp; Concluding Session</b>	
<b>Chairs: N. L. Saini, J. Chen</b>	
17:00-17:30	R. Hennig, <i>Materials Informatics Approaches for the Discovery of Magnetic 2D Materials.</i>
17:30-18:00	A. L. da Rosa, <i>Role of doping and defects on the electronic properties of ZnO.</i>
18:00-18:30	V. Drozd & S. Saxena, <i>Down the memory lane.</i>
18:30-19:00	Organizers & Participants, <i>Concluding Remarks.</i>