



Symposium 2
THEORY AND COMPUTER SIMULATION OF
MATERIALS

CHAIRS:

Dr. Stefano Curtarolo

Duke University, USA

Dr. Romeo de Coss

CINVESTAV - Mérida

Dr. Chris M. Wolverton

Northwestern University, USA

Dr. Marco Buongiorno-Nardelli

North Carolina, USA

Dr. Alejandro Díaz Ortíz

Max-Planck-Institut für Metallforschung Heisenbergstraße

Dr. Edgar Martínez-Guerra

CINVESTAV - Mérida

MONDAY, AUGUST 17

ROOM: TULUM G

(JW MARRIOT)

MORNING SESSION

Session 1: Molecules, clusters and superatoms

Chairperson: Romeo de Coss

S2-1 9:00-9:30 INVITED TALK

SUPERATOMS AND SUPERATOM BASED NANO CLUSTER ASSEMBLED MATERIALS DESIGNER NANO-MATERIALS WITH PRECISE CONTROL OVER PROPERTIES

S. N. Khanna¹

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S2-2 9:30-10:00 INVITED TALK

LARGE CLUSTERS STUDIES WITH DENSITY FUNCTIONAL THEORY

Patrizia Calaminici¹

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S2-3 10:00-10:30 INVITED TALK

HIGH PRESSURE EXTENDED PHASES OF CO₂ AND POSSIBLE IMPLICATIONS

J. A. Montoya¹

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S2-4 10:30-10:45

ELECTRONIC PROPERTIES OF PORPHYRINS INTERACTING WITH GOLD

B.M. Betancourt¹, L.E. Sansores¹

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S2-5 10:45-11:00

CHARACTERIZATION OF METHANOL MONOHYDRATE UNDER PRESSURE: A FIRST PRINCIPLE STUDY

R. E. Dávila-Martínez¹, A. H. Romero Castro¹, R. Caracas²

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11:00-11:30

COFFEE BREAK

11:30-12:30

PLENARY 2

Session 2: Modelling of nanostructures

Chairperson: Noboru Takeuchi

S2-6 12:30-13:00 INVITED TALK

QUANTUM MODELLING OF NANOCRYSTALS, NANOWIRES, AND NANOFILMS

James R. Chelikowsky¹

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S2-7 13:00-13:30 INVITED TALK

MODELLING THE LOW TEMPERATURE DEFORMATION OF CARBON NANOSTRUCTURES AND GRAPHENE

Shuo Chen,^{1,2} Elif Ertekin,² and D. C. Chrzan^{1,2}

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S2-8 13:30-14:00 INVITED TALK

FRICTION AND ADHESION AT THE NANOSCALE

I. Szlufarska¹, Y. Mo¹, Y. Liu¹

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14:00-16:00

LUNCH

16:00-18:30

AFTERNOON SESSION

Session 3: Simulation of chemical reactions and crystal-growth

Chairperson: Edgar Martínez Guerra



S2-9 16:00-16:30 INVITED TALK

A HIERARCHICAL TRANSITION STATE FINDER

A.M. Köster, J.M. del Campo

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S2-10 16:30-17:00 INVITED TALK

SURFACE RADICAL CHAIN REACTION REVISITED: COMPARATIVE INVESTIGATION OF STYRENE AND 2,4-DIMETHYL-STYRENE ON HYDROGENATED Si(001) SURFACE FROM DENSITY FUNCTIONAL THEORY CALCULATIONS

Noboru Takeuchi¹, Yosuke Kanai² and Anabella Selloni³

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S2-11 17:00-17:30 INVITED TALK

THIN FILM GROWTH ON QUASICRYSTALLINE SURFACES

R. D. Diehl¹, K. Pussi², S. Curtarolo³

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S2-12 17:30-18:00 INVITED TALK

MOLECULAR DYNAMICS SIMULATIONS OF NANOSCALE CRYSTAL GROWTH IN PURE Si

Tomorr Haxhimali¹, Dorel Buta¹, Mark Asta¹, Peter W. Voorhees², J. J. Hoyt³

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S2-13 18:00-18:30 INVITED TALK

DYNAMICS OF GROWTH OF COMPLEX MOLECULAR MATERIALS

Aram Amassian¹

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TUESDAY, AUGUST 18

**ROOM: TULUM G
(JW MARRIOT)**

MORNING SESSION

Session 4: Graphene: Electronic structure and Transport

Chairperson: Omar de la Peña

S2-14 9:00-9:30 INVITED TALK

CONTROL OF GRAPHENE ELECTRONIC STRUCTURE THROUGH ADSORBATE INTERACTIONS

Youjian Tang¹, Cheng-Ing Chia¹, Zhaohui Huang¹, and V. H. Crespi¹

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S2-15 9:30-10:00 INVITED TALK

FIRST-PRINCIPLES STUDY OF THE MECHANICAL AND ELECTRONIC PROPERTIES OF GRAPHENE UNDER UNIAXIAL STRAIN

Romeo de Coss¹, Eduardo Cifuentes-Quintal¹, and Edgar Martínez-Guerra^{1,2}

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S2-16 10:00-10:30 INVITED TALK

SEMI-EMPIRICAL TIGHT-BINDING CLUSTER CALCULATIONS OF GRAPHENE AND BN MATERIALS

S. J. Vlaev¹, I. Rodríguez-Vargas¹, R. de Coss², and E. Martínez-Guerra²

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S2-17 10:30-11:00 INVITED TALK

TRANSPORT AND QUANTUM SCATTERING TIMES IN GRAPHENE

X. Hong¹, K. Zou¹ and J. Zhu¹

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11:00-11:30 COFFEE BREAK

11:30-12:30 PLENARY 3

Session 5: Methods and Algorithms for Material Simulations

Chairperson: Stefano Curtarolo

S2-18 12:30-13:00 INVITED TALK

THEORETICAL SPECTROSCOPY OF ORGANIC SEMICONDUCTORS

Leeor Kronik¹

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S2-19 13:00-13:15

DFT SIMULATIONS AT MICRON SCALE AND BEYOND

Gang Lu¹

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S2-20 13:15-13:30

EQUATION OF STATE OF TANTALUM AND IRON FROM FIRST PRINCIPLE

Ljubomir Miljacic¹, Axel van de Walle¹

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S2-21 13:30-13:45

MOLECULAR DYNAMICS STUDIES OF FRICTION IN ALKYL-SILANE AND HYDROALKYL-SILANE COATED MEMS DEVICES

Jose L. Rivera, Oleg A. Mazzyar and Clare McCabe

Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville TN 37235-1604, USA. E-mail: jose.rivera@vanderbilt.edu

S2-22 13:45-14:00

SILK FIBER MECHANICS: MULTI-SCALE MODELLING OF SPIDER SILK

M. Cetinkaya^{1,2}, S. Xiao^{1,3}, F. Graeter^{1,2,3}

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14:00-16:00

LUNCH

16:00-18:30

AFTERNOON SESSION

Session 6: Materials for Energy Applications

Chairperson: Marco Buongiorno

S2-23 16:00-16:30 INVITED TALK

UNDERSTANDING THE MATERIAL THERMODYNAMICS OF TWO-STEP SOLAR THERMOCHEMICAL WATER-SPLITTING CYCLES

B. Meredig¹ and C. Wolverton¹

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S2-24 16:30-17:00 INVITED TALK

AB INITIO MODELLING OF SOLID OXIDE FUEL CELL CATHODES

D. Morgan^{1,2}, Y.-L. Lee¹, J. Kleis³, J. Rossmeisl³

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S2-25 17:00-17:30 INVITED TALK

PREDICTING SOLID-AQUEOUS EQUILIBRIA FOR OPTIMIZED ENERGY STORAGE MATERIALS

K. Persson¹

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S2-26 17:30-18:00 INVITED TALK

NEW HYDROGEN STORAGE MATERIALS VIA COMPUTATION AND EXPERIMENT

Donald J. Siegel^{1,2}

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²Present address: Mechanical Engineering Department, University of Michigan, G.G. Brown Laboratory, 2350 Hayward, Ann Arbor, MI 48109, USA. E-mail: djsiegel@umich.edu

S2-27 18:00-18:30 INVITED TALK

INSIGHTS INTO HYDROGEN DIFFUSION IN METALS AND METAL HYDRIDES FROM FIRST-PRINCIPLES CALCULATIONS

David S. Sholl¹, Shiqiang Hao¹, Lymarie Semidey-Flecha¹, Chen Ling¹, and Sung Gu Kang

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18:30-20:30 POSTER SESSION & COFFEE BREAK

S2-P1

AB INITIO GENERATION OF AMORPHOUS SELENIUM

J. Angel Reyes-Retana¹, Ariel A. Valladares¹

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S2-P2

CHEMICAL ORDERING AND MORPHOLOGY OF AU-PD NANOCCLUS-TERS

J. A. Reyes-Nava¹, J.L. Carrillo², J.F. Rivas-Silva², L. Castañeda-Aviña², and E. Valenzuela¹

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S2-P3

AB-INITIO STUDY OF THE POLYCHLORINATED BIPHENYLS: CORRE-LATION BETWEEN ELECTRONIC STRUCTURE AND LIPOPHILICITY

C.M. Ramos-Castillo¹, E. Martínez-Guerra^{1,2}, E. Cifuentes-Quintal¹, and R. de Coss¹

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S2-P4

INFLUENCE OF LI COVERAGE ON HYDROGEN ADSORPTION ON SINGLE WALL CARBON NANOTUBES

Eduardo Rangel^a, Gregorio Ruiz-Chavarria^{a,b}, L. F. Magana^a

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S2-P5

UNIDIMENSIONAL SILVER NANOSTRUCTURES N-ALKYLTHIOL: THEORETICAL ANALYSIS OF REACTIVITY

M. E. Fernández-García¹ and C. E. Gutiérrez-Wing¹

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S2-P6

ADSORPTION OF CARBON DIOXIDE (CO₂) NAD METHANE (CH₄) ON THE SURFACE OF A TITANIUM-GRAPHENE SYSTEM WITH HIGH METAL COVERAGE

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S2-P7

COOPER, PHOSPHORUS AND OZONE INTERACTION WITH THE C₆₀-20 FULLERENE SECTION IN A SILICON SUBSTRATE

Alejandro Valderrama¹, L. F. Magana¹, Gregorio Ruiz-Chavarría^{1,2}, Eduardo Rangel¹

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S2-P8

FIRST PRINCIPLE CALCULATION OF THE INTERACTION OF THE SILICON SURFACE (001)_c(2×4) WITH FLUOR AND CHARGE DISTRIBUTION

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S2-P9

THE NITRIC OXIDE ADSORPTION ON GOLD ATOM. A COMPARATIVE AN INITIO MRCI AND MRPT2 STUDIES

O. Olvera-Neria¹, E. Poulain-García¹, V. Bertín-Mardel², V.H. Uc-Rosas¹.

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S2-P10

MOLECULAR SIMULATION OF THIOL-FUNCTIONALIZED CARBON NANOTUBES

R. Rivera¹, R. Esparza², R. Pérez², E. Rubio-Rosas¹ and V. Rodríguez-Lugo¹

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S2-P11

(0 0 1) IDEAL-SURFACE BAND STRUCTURE FOR THE SERIES OF CU-BASED CHALCOPYRITES TYPE Cu₂Bi₂(VI)₂

H. Tototzintle-Huitle¹, F. Puch¹, J.J. Araiza¹ and R. Baquero²

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S2-P12

THEORETICAL CALCULATIONS OF THE GEOMETRIC AND ELECTRONIC STRUCTURES OF CHLORAPATITE, FLUORAPATITE AND HYDROXYAPATITE

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S2-P13

COMPARATIVE STUDY OF NONPROPORTIONALITY OF INORGANIC SCINTILLATORS AND ELECTRONIC BAND STRUCTURES

W. Setyawan¹, R. M. Gaume², S. Lam², R. S. Feigelson², and S. Curtarolo¹

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S2-P14

STUDY OF THE ELECTRONIC STRUCTURE OF CERIUM-ZIRCONIUM-OXIGEN Ce_{0.5}Zr_{0.5}O₂

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S2-P15

CALCULATING THE VIBRATIONAL DENSITY OF STATES OF AMORPHOUS Si_{0.5}Ge_{0.5}

L. M. Mejía Mendoza¹, R. M. Valladares Mc Nelis², Ariel A. Valladares¹.

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S2-P16

EXCESS OF LOW FREQUENCY VIBRATIONAL MODES AND GLASS TRANSITION: A MOLECULAR DYNAMICS STUDY IN LENNARD-JONES SYSTEMS AT CONSTANT PRESSURE

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S2-P17

AB-INITIO STUDY OF THE E_{2g} PHONON MODE IN GRAPHENE UNDER BIAXIAL STRAIN

Eduardo Cifuentes-Quintal¹, Edgar Martínez-Guerra^{1,2}, and Romeo de Coss¹

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S2-P18

THEROTICAL SUDY OF Fe₄-(Benzene) *m*, *m* ≤ 4

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S2-P19

STUDY OF THE COORDINATION MODES FOR Fe_n-(Benzene) *m*, *n*=1,2; *m* ≤ *n*

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S2-P20

YFe₅ MAGNETIC MOMENT BEHAVIOR UNDER EXTERNAL HYDROSTATIC PRESSURE

D. Lozano¹, J.T. Elizalde Galindo¹, G. Rivas Valles¹, S. Terrazas Porras¹, J. Sáenz Villela



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WEDNESDAY, AUGUST 19

**ROOM: TULUM G
(JW MARRIOT)**

MORNING SESSION

Session 7: New Methods for Modelling Alloys

Chairperson: Chris Wolverton

S2-28 9:00-9:30 INVITED TALK

THE PREDICTION OF CRYSTAL STRUCTURE BY COMBINING MACHINE LEARNING KNOWLEDGE METHODS WITH FIRST PRINCIPLE ENERGY METHODS

G. Ceder¹

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S2-29 9:30-10:00 INVITED TALK

CHASING EXOTIC BINARY ALLOY COMPOUNDS: THE NECESSARY SYNERGY OF CLUSTER EXPANSION AND HIGH-THROUGHPUT METHODS

Stefano Curtarolo¹, Gus L.W. Hart², Ohad Levy^{1*}

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S2-30 10:00-10:30 INVITED TALK

HIGH-THROUGHPUT AND CLUSTER EXPANSION SEARCH FOR NEW MAGNESIUM ALLOYS: EXAMPLE OF Li-Mg

Gus L.W. Hart¹, Richard Taylor and Stefano Curtarolo²

¹Brigham Young University

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S2-31 10:30-11:00 INVITED TALK

MATERIALS CARTOGRAPHY IN HCP CRYSTALS: ELASTIC INTERACTIONS

Alejandro Díaz Ortiz¹

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11:00-11:30 COFFEE BREAK

11:30-12:30 PLENARY 4

Session 8: Thermodynamic and mechanical properties of materials

Chairperson: Alejandro Díaz

S2-32 12:30-13:00 INVITED TALK

FIRST-PRINCIPLES CALCULATIONS OF FREE ENERGIES OF UNSTABLE PHASES

Vidvuds Ozolins¹

¹Department of Materials Science and Engineering, University of California, Los Angeles, California, 90095-1595, USA. E-mail: vidvuds@ucla.edu

S2-33 13:00-13:30 INVITED TALK

THE ACCURACY OF FIRST PRINCIPLE METHODS IN PREDICTING THERMODYNAMIC PROPERTIES OF METALS

T. Hickel, B. Grabowski, F. Körmann, A. Dick, J. Neugebauer

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S2-34 13:30-14:00 INVITED TALK

THE HAMMON POSTULATE IN THE STUDY OF MECHANICAL BEHAVIOR

M. E. Eberhart¹, T. E. Jones¹

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14:00-16:00 LUNCH

16:00-18:30 AFTERNOON SESSION

Session 9: Simulation of Nanodevices

Chairperson: Vincent Crespi

S2-35 16:00-16:30 INVITED TALK

FIRST PRINCIPLES CALCULATIONS OF CHARGE MOBILITY AND HEAT TRANSPORT: A PRACTICAL TOOL-SET FOR THE EFFICIENT DESIGN OF NOVEL MATERIALS AND DEVICES FOR NANOELECTRONIC APPLICATIONS

Marco Buongiorno Nardelli¹

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S2-36 16:30-17:00 INVITED TALK

MULTISCALE SIMULATIONS AND DESIGN OF NANO MATERIALS AND NANODEVICES

J. Bernholc^{1,2}, W. Lu,^{1,2} F. Ribeiro,¹ K. Saha,² J. Jiang,¹ V. Ranjan,¹ L. Yu,¹ V. Meunier,² and M. Buongiorno Nardelli^{1,2}

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S2-37 17:00-17:30 INVITED TALK

THEORETICAL NANOSCIENCE AND COMPUTATIONAL MODELLING AT LENGTH SCALES RELEVANT TO EXPERIMENT

Vincent Meunier¹

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S2-38 17:30-18:00 INVITED TALK

NON-EQUILIBRIUM ELECTRON TRANSPORT IN DRY DNA

C. D. Pemmaraju, I. Rungger, A. Rocha and S. Sanvito

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S2-39

18:00-18:30 INVITED TALK

AUGER RECOMBINATION RATES IN NITRIDES FROM FIRST PRINCIPLES

Patrick Rinke, Kris T. Delaney, Chris G. Van de Walle
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18:30-20:30 POSTER SESSION & COFFEE BREAK

S2-P21

DETERMINATION OF THE GROUND STATE OF THE Al-Si-Sr SYSTEM BY FIRST-PRINCIPLES CALCULATIONS

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S2-P22

MOLECULAR DYNAMICS-AB INITIO STUDY OF LIQUID Al -4.8 at.% Si

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S2-P23

A NANO-SYRINGE FOR THE TRANSPORT OF THIN WATER FILLS ACROSS CARBON NANOTUBES MEMBRANES

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S2-P24

LOW-ENERGY ELECTRON DIFFRACTION STUDIES OF THE STRUCTURES OF FULLERENES ON CLOSE-PACKED METAL SURFACES

H. I. Li¹, H. Shin¹, K. Pussi², L. W. Bruch, R. D. Diehl¹
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S2-P25

BIOMOLECULAR STORAGE CAPACITIES OF CNT'S: INSIGHTS FROM DFT

Aned de Leon¹, Alvaro Posada-Amarillas¹ and Abraham F. Jalbout¹
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S2-P26

NANOTUBES AS FREE RADICAL "SPONGES" IN DNA: A THEORETICAL PROPOSAL

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S2-P27 INVITED TALK

CALCULATED I-V CURVES FOR OLIGOANILINES AND F-OPE (FLUORO OLIGO PHENYLENE ETHYNYLENE) USING NON-EQUILIBRIUM GREEN FUNCTION FORMALISM (NEGF AND DFT)

L. Serrato¹, M. Gallo¹, M.T. Romero² y D. Glossman-Mitnik³
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S2-P28

THEORETICAL STUDY OF THE ELECTRONIC STRUCTURE IN ORGANIC MOLECULES AND THE APPLICATIONS IN PHOTOVOLTAIC DEVICES

R. M. Gutiérrez-Pérez¹, N. Flores-Holguín², N. Sánchez-Bojorge², D. Glossman-Mitnik², L.M. Rodríguez-Valdez¹.
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S2-P29

THIAIAZOLES AS ORGANIC PHOTOVOLTAIC MATERIALS: A THEORETICAL PROPERTIES STUDY

N. Sánchez-Bojorge¹, L.M. Rodríguez-Valdez², D. Glossman-Mitnik¹ and N. Flores-Holguín¹
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S2-P30

SIMULATION AND STUDY OF THE INFLUENCE OF THE BUFFER INTRINSIC LAYER, BACK SURFACE FIELD, DENSITY OF INTERFACE DEFECT AND RESISTIVITY OF P-TYPE SILICON SUBSTRATE ON THE HIT (HETEROJUNCTION WITH INTRINSIC THIN LAYER) SOLAR CELL

J. Heo¹, V. Ai¹, H. Choi¹, Y. Kim¹, N. Lakshminarayanan², J. Yi¹
¹School of Information and Communication Engineering, Sungkyunkwan University, 300. Chungchun-dong, Jangan-Gu, Suwon-City, Kyunggi-Do, 440-746, Republic of Korea. ²Department of Physics, Madras Christian College, Chennai 600059, India. Email: fbc@korea.com

S2-P31

NONLINEAR PULSE PROPAGATION THROUGH A SEMICONDUCTOR PERIODIC STACK

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S2-P32

ON THE POSSIBLE LIGAND POINTS ON MAYE BLUE

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S2-P33

STUDY OF ABSORPTION AND REFRACTIVE INDEX GRATINGS ON THE BEAM COUPLING IN BTO EMPLOYING A VECTOR APPROACH

M.A. González-Trujillo^{1,3}, I. Casar², J. Murillo³, R. Farías³

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S2-P34

PREDICTION OF CRITICAL POINTS IN TERNARY MIXTURES OF ALKANES + WATER

J. Barajas-Fernández¹, M.A. Olán-Acosta¹, L.L. Díaz-Flores¹, J.G.F. Rivera-Trejo¹, Y.E. Hernández-Cardeño¹, E.D. Bolaina-Lorenzo¹

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S2-P35

SIMULACIÓN DE FRACTURA EN MATERIALES FRÁGILES A LA ESCALA NANOMÉTRICA

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S2-P36

SURROGATE MODELLING OF WATER UPTAKE FOR BIODEGRADABLE POLYMERS

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S2-P37

MODELLING OF LASER CO₂ SURFACE TREATMENT OF ASTM F75 COBALT BASE ALLOY

F. Cepeda-Rodríguez¹, J. L. Acevedo-Davila¹, M.A.L. Hernández-Rodríguez², L.E. Ramírez-Vidaurre³, Y. Cepeda-Rodríguez³.

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S2-P38

THEORETICAL ANALYSIS OF THE DISFUNCIONALES PROCESSES OF ELECTRIC GENERATORS

A. Cueto-Hernández¹, L.A. García-Serrano², R. Radillo-Ruiz², J.M. Hernández-Enriquez²

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S2-P39

HEAT TRANSFER STUDY IN TOOL STEEL AISI H13 DURING THERMAL FATIGUE TESTS

M.A. Quiñones Salinas¹, R.D. Mercado Solís¹, M. Hernández Rodríguez¹, A. Juárez Hernández

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THURSDAY, AUGUST 20

ROOM: TULUM G

(JW MARRIOT)

MORNING SESSION

Session 10: Simulation of Magnetic Materials

Chairperson: Oracio Navarro

S2-40 9:00-9:30 INVITED TALK

MAGNETISM BASED ON P-ORBITALS

P. Bogusławski^{1,2}, O. Volnianska¹

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S2-41 9:30-10:00 INVITED TALK

FERROMAGNETISM IN MgO_{1-x}N_x: DENSITY-FUNCTIONAL CALCULATIONS

M. Ležaić, Ph. Mavropoulos and S. Blügel

Institut für Festkörperforschung, Forschungszentrum Jülich, Leo-Brandtstr, 52425 Jülich, Germany. E-mail: m.lezaic@fz-juelich.de

S2-42 10:00-10:30 INVITED TALK

DENSITY FUNCTIONAL STUDY OF THE HALF-METALLIC FERROMAGNETISM IN Co-BASED HEUSLER ALLOYS Co₂MSn (M = Ti, Zr, Hf) USING LSDA and GGA

Aaron Aguayo¹, Gabriel Murrieta¹

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S2-43 10:30-11:00 INVITED TALK

AB INITIO CALCULATIONS ON MIXING AND MAGNETISM IN SURFACE ALLOYS

Shobhana Narasimhan, Madhura Marathe and Mighfar Imam

Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore 560064, India. E-mail: shobhana@jncasr.ac.in

11:00-11:30

COFFEE BREAK

11:30-12:30

PLENARY 5



Session 11: Complex Materials

Chairperson: Rafael Baquero

S2-44 12:30-13:00 INVITED TALK

RARE EARTHS TO Pnictides: RECENT THEORY/COMPUTATIONAL INSIGHTS

B. N. Harmon¹, Y. Lee¹, S. E. Hahn¹

¹Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, IA, 50011, USA. E-mail: harmon@ameslab.gov

S2-45 13:00-13:30 INVITED TALK

X-RAY ABSORPTION IN IRON ARSENIDE RARE EARTH OXIDES: THEORY AND EXPERIMENT

J. Mustre de León^a, A. Bianconi^b, N. Saini^b, J. Lezama Pacheco^a

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S2-46 13:30-14:00 INVITED TALK

FIRST PRINCIPLE STUDY OF THE ELECTRONIC STRUCTURE AND PHONON PROPERTIES ON MANGANITES

O. De la Peña-Seaman¹, R. Heid¹, and K.-P. Bohnen¹.

¹Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O. Box 3640, D-76021 Karlsruhe, Germany. E-mail: seaman@ifp.fzk.de

14:00-16:00 LUNCH

16:00-18:30 AFTERNOON SESSION

Session 12: Electronic correlation and superconductivity

Chairperson: José Mustre de León

S2-47 16:00-16:30 INVITED TALK

EXTENDED LDA+U+V APPROACH FOR COVALENTLY BONDED SYSTEMS

Vivaldo Leiria Campo, Jr.¹ and Matteo Cococcioni²

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S2-48 16:30-17:00 INVITED TALK

ELECTRONIC CORRELATIONS AND DISORDER IN FeMo DOUBLE PEROVSKITE COMPOUNDS

O. Navarro¹ and M. Avignon²

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S2-49 17:00-17:30 INVITED TALK

MAGNETIC SUSCEPTIBILITY IN THE ONE DIMENSIONAL DOUBLE AND SUPER-EXCHANGE MODEL

O. Navarro¹, E. Vallejo¹, J.R. Suárez¹ and M. Avignon²

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S2-50 17:30-18:00 INVITED TALK

SUPERCONDUCTOR-SEMICONDUCTOR INTERFACES

Rafael Baquero¹

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S2-51 18:00-18:15

CaLi₂ AT HIGH PRESSURE: CRYSTALLOGRAPHY, ELECTRONIC STRUCTURE, PHONONS AND SUPERCONDUCTIVITY

Y. Xie^{1,2}, A. Oganov², and Y.M. Ma¹

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18:15-18:30

FINAL REMARKS