

# Symposium N

WEDNESDAY OCTOBER 11<sup>TH</sup>



## 8:15 A.M. – 10:15 A.M. – ORAL SESSION N1

Chairperson: Petrili, H. M.

Room: FEI Company

8:15-8:45 A.M. MODELING MATERIALS: METHODOLOGIES AND APPLICATIONS (N554,Invited) Marco A. Chaer Nascimento (IQ-UFRJ)

8:45-9:00 A.M. INVESTIGATION OF CHANNELING IN CARBON NANOTUBES THROUGH MOLECULAR DYNAMICS SIMULATION (N503) Cássio Stein Moura (UFRGS) and Livio Amaral (UFRGS)

9:00-9:15 A.M. MOLECULAR DYNAMICS SIMULATION OF IONIC LIQUIDS POLYMER ELECTROLYTES (N506) Mauro C. C. Ribeiro (IQ - USP) and Luicano T. Costa (IQ - USP)

9:15-9:30 A.M. HYDROGENATION OF ETHENE CATALYZED BY H-ZSM-5 MICROPOROUS MOLECULAR SIEVE: A THEORETICAL STUDY (N510) Castro, Elton Santos.

9:30-9:45 A.M. CALCULATION OF ELECTRONIC,STRUCTURAL AND ELASTIC PROPERTIES OF FE<sub>2</sub>MN<sub>3</sub> HEUSERL INTERMETALLIC COMPOUND (N512) Ariana de Campos (Unicamp), Adelino Aguiar Coelho (Unicamp), Sergio Gama (Unicamp), Laudemir Carlos Varanda (Unesp), Miguel Jafelicci Junior (Unesp), Alisson Almeida Bueno (Unesp), Momotaro Imaizumi (Unesp), Luana Caron (Unicamp) and Julio Ricardo Sambrano (Unesp)

9:45-10:00 A.M. ELECTRONIC STRUCTURE CALCULATIONS OF CAROTENOIDS IN THE BURITI OIL/POLYSTYRENE COMPOSITES (N515) Maria José A. Sales (IQ/UnB), Geraldo Magela e Silva (IF/UnB), Artemis Ceschin Marti (IQ/UnB), Jussara Angélica Durães (IQ/UnB), Alessandra F. A. Vilela (IF/UnB), João B. L. Martins (IQ/UnB) and Ricardo Gargano (IF/UnB)

10:00-10:15 A.M. METHODOLOGY COMPARED OF THE SELF-CONSISTENT BAND STRUCTURE CALCULATIONS WERE PERFORMED FOR THE NITRIDES (N516) Eduardo Angst Tonetto (URI) and Antonio vanderlei dos Santos (URI) ■



## 10:15 A.M. - 10:30 A.M. – COFFEE BREAK



## 10:30 A.M. – 12:30 P.M. – ORAL SESSION N2

Chairperson: Ricardo Longo

Room: FEI Company

10:30-11:00 A.M. APPLICATIONS OF EMPIRICAL, SEMI-EMPIRICAL, AB-INITIO AND BAND THEORETICAL MODELS TO INTERDISCIPLINARY PROBLEMS IN

PHYSICAL CHEMISTRY AND MATERIAL SCIENCE. (N575, Invited). Carlton Taft (DMF -CBPF)

11:00-11:15 A.M. INDIVIDUAL CONTRIBUTION OF THE MATRIX AND TRIGLYCERIDES TO BANGAP OF BURITI OIL: POLYSTYRENE BLENDS (N522) Jussara A. Durães (UnB); Maria José A. Sales (UnB); Elton A. Castro (UnB); João Batista Lopes Martins (UnB); Geraldo Magela (UnB); Ricardo Gargano; Artemis Marti Ceschin (UnB).

11:15-11:30 A.M. BLUE-GREEN AND RED PHOTOLUMINESCENCE IN CaTiO<sub>3</sub>:Sm (N527) Fábio S. De Vicente (USP), Valmor R. Mastelaro (USP), Alberthmeiry T. de Figueiredo (Ufscar), Valeria M. Longo (Ufscar), Sergio de Lazaro (Ufscar), Antônio C. Hernandez (USP), Máximo Siu Li (USP), José A. Varela (UNESP) and Elson Longo (UNESP)

11:30-11:45 A.M. THEORETICAL STUDY OF THE FE/ZSM-5 ZEOLITE (N545) Aguinaldo Robinson de Souza (UNESP), Nelson Henrique Morgon (UNICAMP) and Julio Ricardo Sambrano (UNESP)

11:45-12:00 P.M. FRICTION IN MAGNETIC DEVICES – A MOLECULAR DYNAMIC STUDY (N546) Marcella Rapini Braga (UFMG), Bismarck Vaz da Costa (UFMG) and Rodrigo Alves Dias (UFMG)

12:00-12:30 P.M. AB INITIO METHODS AND GROUND-STATE PROPERTIES OF MATERIALS (N579, Invited) Kuhnén, Carlos Alberto (UFSC). ■



## 12:30 P.M. – 2:00 P.M – LUNCH



## 2:00 P.M. – 2:45 P.M – PLENARY LECTURE

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## 2:50 P.M. – 4:20 P.M. – ORAL SESSION N3

Chairperson: Sergio de Lazaro

Room: FEI Company

2:50-3:20 P.M. EXPERIMENT AND THEORY IN CONCERT. SEARCHING MOLECULAR CONDUCTORS WITH MULTIFACETED PROPERTIES: THE CASE OF MO<sub>3</sub>S<sub>7</sub> TRINUCLEAR CLUSTERS WITH OUTER DITHIOLATE LIGANDS (Invited, N581) Victor Polo (Göteborg University, Sweden), R. Llusar (Universitat Jaume I), S. Triguero (Universitat Jaume I) and Juan Andrés (Universitat Jaume I).

3:20-3:35 P.M. CHARGE AND SPIN DISTRIBUTION IN (III,V)-MN FERROMAGNETIC MULTILAYERS (N547) I. C. da Cunha Lima (UERJ), E. F. da Silva Jr. (UFPE), G. M. Sipahi (USP), L. M. R. Scolfaro

(UFPE/USP), I. S. P. Marin (USP) and S. C. P. Rodrigues (UFPE)



10:45 A.M. - **CLOSING PLENARY SESSION**

3:35-3:50 P.M. DESIGN OF NEW POROUS MATERIALS FOR NATURAL GAS STORAGE **(N556)** Ricardo Luiz Longo (UFPE) and Elisa Soares Leite (UFPE).

3:50-4:05 P.M. COMPUTATIONAL GRAPHIC SIMULATION OF MORE THAN THREE COMPONENTS MIXTURES EQUATION ADJUSTMENT TO THE DEVELOPMENT OF NEW MATERIALS **(N559)** José Vidal Nardi (CEFET/SC)

4:05-4:20 P.M. NUMERICAL SIMULATION OF OSTWALD RIPENING OF PRECIPITATES IN REACTION CONTROLLED GROWTH **(N567)** Gustavo Lotici Hennig (UNIJUI), Zacarias Eduardo Fabrin (UNIJUI) and Gerson Feldmann (UNIJUI) ■



4:20 P.M. – 4:40 P.M. – **COFFEE BREAK**



5:50 P.M. – 7:00 P.M. – **PLENARY SESSION**



20:30 P.M. ✦ **Conference Dinner** ✦  
Local: Swimming Pool Lounge

## THURSDAY, OCTOBER 12



8:15 A.M. – 10:15 P.M. – **ORAL SESSION N4**  
Chairperson: Carlton Taft  
Room: FEI Company

8:15-8:45 A.M. COMPUTER SIMULATIONS THROUGH AB INITIO ELECTRONIC STRUCTURE CALCULATIONS, **(N580,Invited)** Petrijli, H. M.

8:45-9:00 A.M. OPTICAL PROPERTIES AND COMPUTER MODELLING OF RE DOPED BISMUTH GERMANATE **(N568)** Geane da Cruz Santana (UFS), Mario Ernesto Giroldo Valerio (UFS), Zelia Soares Macedo (UFS) and Robert Adam Jackson (University of Keele)

9:00-9:15 A.M. INTERCHAIN INTERACTION EFFECTS ON POLARON-BIPOLARON TRANSITION ON CONDUCTING POLYMERS **(N577)** Geraldo Magela e Silva (UnB) and José Rildo de Oliveira Queiroz (UnB)

9:15-9:30 A.M. DISCUSSION (Chair: Martins, J. B. L. and Sambrano, J. R.) ■



9:30 A.M. - 10:45 A.M. - **POSTER SESSION PN1**  
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10:15 A.M. - 10:30 A.M. – **COFFEE BREAK**