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ABSTRACT BOOK

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DIFFUSION IN SOLIDS AND LIQUIDS - DSL2019**

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DSL104

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Diffusion of Gases in Glassy Polymers Determined with PGSE NMR

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The transport of gases in polymer membranes has wide implications in diverse industrial applications and advancing knowledge in this area could facilitate the design of membranes with improved performance [1]. In this regard, nuclear magnetic resonance, NMR, is able to provide a wealth of information on different kinds of samples and processes at molecular level. Thus, NMR allows the study of small molecules dynamics in a medium and correlation of the results with its physicochemical properties [2].

In this communication, measurements of diffusion coefficients of pure and mixed gases ($^{13}\text{CO}_2$, CH_4 , C_2H_4) in amorphous polymers (polyimide, polycarbonate) below the glass transition temperature with multinuclear pulsed gradient spin echo (PGSE) NMR are described. In addition, NMR spin-lattice and spin-spin relaxation times, and solubility coefficients are determined to characterize the behavior of sorbed gases and the transport phenomenon in glassy polymer membranes. The relaxation times results show evidence of only one type of population of sorbed gas molecules in the membranes. The solubility coefficients determined with ^1H and ^{13}C NMR spectroscopy are in good agreement with those in the literature. It is observed that the diffusivity of hydrocarbons in the polymers studied exhibited a non-Fickian behavior, while the diffusion of $^{13}\text{CO}_2$ followed Fick's laws. In gas mixtures, the presence of highly condensable gases ($^{13}\text{CO}_2$ and C_2H_4) in the membranes, even at low concentration (partial pressure < 3 bar), changes the mobility of polymer chains increasing the diffusion coefficient of CH_4 .

[1] M. Galizia, W.S. Chi, Z.P. Smith, T.C. Merkel, R.W. Baker, B.D. Freeman. *Macromolecules*, 50, 7809 (2017).

[2] L. Garrido, J. Guzmán. *J. Phys. Chem. B*, 116, 6050 (2012).

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DSL119

Dr. Sara Faiz Hanna Tasfy

American University of Ras Al Khaimah,
United Arab Emirates

HEAT AND MASS TRANSFER IN POROUS MEDIA (SS7) Chairs: Prof. Joao Delgado Prof. Antonio G.B. de Lima			
8.30-9.00 OPENING TALK VIP048 Prof. Antonio G.B. de Lima Federal University of Campina Grande, Brazil ON THE MODELING OF DRYING PROCESS IN INDUSTRIAL TUNNEL DRYER A.G.B. de Lima	DIFFUSION PROCESSES UNDER STRAINING (SS6) Chairs: PD Dr. Sergiy Divinski Dr. Vladimir Esin Dr. Laure Martinelli Dr. Cécilie Duhamel	NANO/BIO MATERIALS SYNTHESIS, CHARACTERIZATION, MODELING AND APPLICATIONS (SS9) Chair: Prof. A. Shokuhfar	DIFFUSION AND IONIC CONDUCTIVITY IN INORGANIC COMPOUNDS (SS5) Chair: Prof. Manfred Martin (Part 2)
9.00-9.30 INVITED TALK VIP152 Prof. Anthony G. Straatman Western University, Canada A MULTI-LEVEL APPROACH FOR SIMULATION OF STORAGE AND RESPIRATION OF PRODUCE M. Elhalwagy, N. Dyck and A. G. Straatman			
9.30-10.00 INVITED TALK VIP084 Prof. Jozef Kačur SvF STU, Bratislava, Slovakia NUMERICAL MODELING OF HEAT AND MASS TRANSPORT WITH INNER HEAT EXCHANGE IN UNSATURATED POROUS MEDIA Jozef Kačur, Patrik Mihala	9.30-10.00 OPENING TALK VIP022 Dr. Cecilia Duhamel MINES ParisTech, PSL Research University, France PLASTICITY-ENHANCED DIFFUSION OF Cr in Ni J. Nguejio, B. Chetroui, J. Crépin, C. Duhamel, V. Esin, C. Guerre, F. Jomard, M. Maisonneuve	9.30-10.00 INVITED TALK VIP095 Dr. Narguess Nemati Yonsei University, Korea EXTREMELY DURABLE MULTILAYERED COATING DESIGN PRINCIPLE, A NEW PARADIGM TOWARD HIERARCHICAL SURFACE PROTECTION	9.30-10.00 INVITED TALK DSL204 Dr. Andreas Falkenstein RWTH Aachen University, Germany TRANSPORT KINETICS OF HYDROGEN PERMEABLE LANTHANUM TUNGSTATE A. Falkenstein, M. Martin
10.00-10.20 COFFEE BREAK			
10.20-10.50 INVITED TALK VIP085 Prof. Alfio Grillo Politecnico di Torino, Italy MECHANICAL AND FLOW PROPERTIES OF FIBRE-REINFORCED, HYDRATED BIOLOGICAL TISSUES UNDERGOING REMODELLING A. Grillo, S. Di Stefano	10.20-10.50 INVITED TALK VIP041 Prof. Dominique Mangelinck IM2NP, Faculté des Sciences et Techniques, France STRAIN IN SILICIDE FORMATION AND STABILITY D. Mangelinck	10.20-10.50 INVITED TALK DSL247 Prof. Noorhana Yahya Universiti Teknologi PETRONAS, Malaysia DFT STUDY OF ADSORPTION OF H₂, N₂ AND CO₂ ON THE SURFACE OF HEMATITE NANOCATALYSTS FOR GREEN UREA SYNTHESIS Noorhana Yahya, Bilal Alqasem	10.20-10.40 DSL167 Ms. Selma Rabhi Aix-Marseille Université (AMU), France EFFECT OF THE THICKNESS ON THE SOLID STATE REACTION OF Ni / GaAs AND PHASE FORMATION KINETICS S. Rabhi, C. Perrin-Pellegrino, M.C. Benoudia, K. Hoummada
10.50-11.20 INVITED TALK VIP051 Prof. Dieter Freude Universität Leipzig, Germany TWO-REGION MODEL AND MAS PFG NMR DIFFUSOMETRY D. Freude, J. Kärger	10.50-11.20 INVITED TALK VIP039 Dr. Tilmann Hickel Max-Planck-Institute of Iron Research, Germany PRECIPITATE-INDUCED NONLINEARITIES OF SOLUTE DIFFUSION IN AL-BASED ALLOYS Tilmann Hickel, Ankit Gupta, Jörg Neugebauer, Vladislav Kulitcki, Bengü Tas Kavakbasi, Yulia Buranova, Gerhard Wilde and Sergiy V. Divinski	10.50-11.20 INVITED TALK DSL089 A/Prof. Bryan B. Pajarito University of the Philippines, Philippines GRAPHITE NANOPlatelets FROM WASTE CHICKEN FEATHER B.B. Pajarito, A.J.B. Belarmino, R.M.R. Calimbas, J.R.B. Gonzales, M.N. Acda	10.40-11.00 DSL161 Mr. Christian Schwab RWTH Aachen University, Germany BULK AND GRAIN BOUNDARY DIFFUSION OF Li IN DENSE LiMn₂O₄ PELLETS BY MEANS OF 6Li-tracer EXPERIMENTS C. Schwab, M. Martin

11.20-11.50	11.20-11.50	11.20-11.40	11.00-11.20
<p>INVITED TALK VIP047 Prof. Isabel Malico Universidade de Évora, Portugal NUMERICAL SIMULATION AND OPTIMIZATION APPLIED TO POROUS MEDIA: A REVIEW I. Malico, S. Cavaleiro Costa</p>	<p>INVITED TALK VIP035 Prof. Zhenbo Wang Institute of Metal Research Chinese Academy of Sciences (IMR CAS), China DIFFUSION IN NANO-LAMINATED METALS WITH HIGHER THERMAL STABILITY Z.B. Wang, S.L. Xie, Z.P. Luo, S. Divinski and K. Lu</p>	<p>DSL104 <u>Dr. Leoncio Garrido</u> Instituto de Ciencia y Tecnología de Polímeros, Spain DIFFUSION OF GASES IN GLASSY POLYMERS DETERMINED WITH PGSE NMR <u>L. Garrido, J. Guzmán</u></p>	<p>DSL088 <u>Dr. Cristian Ravariu</u> University Polytechnic of Bucharest, Romania AN APPROPRIATE DIFFUSION PROCESS CHANGES THE DESTINY OF A PLANAR-NOTHING ON INSULATOR (p-NOI) NANOELECTRONIC DEVICE C. Ravariu, C. Părvulescu, E. Manea, F. Babarada</p>
11.50-12.10	11.50-12.20	12.00-12.20	11.40-12.00
<p>DSL118 Mr. Patrik Mihala SvF STU, Bratislava, Slovakia NUMERICAL MODELING OF HEAT AND MASS TRANSPORT WITH INNER HEAT EXCHANGE IN UNSATURATED POROUS MEDIA J. Kačur, P. Mihala</p>	<p>INVITED TALK VIP052 <u>Dr. Maylise Nastar</u> University Paris-Saclay, France MODELING OF NANOSCALE ELASTO-DIFFUSION IN Si, Fe(Cr) AND Ni(Si) DILUTE ALLOYS Fabien Bruneval, Luca Messina, Thomas Schuler, Maylise Nastar</p>	<p>DSL130 <u>Prof. Fominykh Andrew</u> Ben-Gurion University of the Negev, Israel ADSORPTION OF TRACE ATMOSPHERIC GASES IN ATMOSPHERIC BOUNDARY LAYER BY DUST AEROSOL PARTICLES EMITTED FROM ARID SOURCE AREAS Boris Krasovitov, Itzhak Katra, Tov Elperin, Andrew Fominykh</p>	<p>DSL188 <u>Mr. Andrey Gladilin</u> Prokhorov General Physics Institute of the Russian Academy of Sciences, Russia THE INFLUENCE OF IRON THERMAL-DIFFUSION-BASED DOPING ON THE SPATIAL DISTRIBUTION OF LUMINESCENCE INTENSITY IN ZnSe AND ZnS CRYSTALS A.A. Gladilin, V.P. Kalinuskin, O.V. Uvarov, N.N. Il'ichev, N.A. Timofeeva, E.M. Gavrischuk, S.I. Chentsov, V.S. Krivobok</p>
12.10-12.30	12.20-12.40	12.20-12.40	12.00-12.20
<p>DSL242 <u>Dr. Hossein Davarzani</u> French Geological Survey (BRGM), France EXPERIMENTAL AND MODELING STUDY OF TWO PHASE HEAT AND MASS TRANSPORT DURING MICROWAVE HEATING REMEDIATION OF CONTAMINATED SOILS H. Davarzani, O. Ali Djigo, S. Colombano, Y. Menard</p>	<p>DSL235 <u>Dr. Andrei V. Nazarov</u> National Research Nuclear University MEPhI «Moscow Engineering Physics Institute», Russia KINETICS OF SEGREGATION FORMATION NEAR THE EDGE DISLOCATION IN bcc IRON A.V. Nazarov and A.A. Gusev</p>	<p>DSL184 <u>Prof. Micha Polak</u> Ben-Gurion University of the Negev, Israel COMPREHENSIVE MODELING OF Cu-Ni NANO-PHASE DIAGRAMS BASED ON CORRECTED COHESION AND COORDINATION-DEPENDENT BOND ENERGIES M. Polak and L. Rubinovich</p>	<p>DSL240 <u>Mr. Christoph Tietz</u> University of Vienna, Austria BEAM-INDUCED DYNAMICS IN OXIDE GLASSES C. Tietz, K. Holzweber, T. Fritz, M. Legenstein, B. Sepiol</p>
12.30-12.50	12.40-13.10	12.40-13.00	
<p>DSL175 <u>Prof. Nafisah Osman</u> Universiti Teknologi MARA, Malaysia FABRICATION OF COMPOSITIONALLY GRADIENT ANODE FUNCTIONAL LAYERS FOR PROTON CONDUCTING FUEL CELL AT INTERMEDIATE TEMPERATURES N. Osman, L.A. Malik, N.S.M Affandi, O.H. Hassan and A.M.M. Jani</p>	<p>CLOSING TALK VIP037 <u>Dr. Laure Martinelli</u> CEA/DPC/SCCME, France EXPERIMENTAL STUDY OF Cr TRACER DIFFUSION IN Ni(-Cr) AND APPLICATION TO Ni-Cr OXIDATION T. Gheno, C. Desgranges, L. Martinelli</p>	<p>DSL100 <u>Dr. Olga Molodtsova</u> Deutsches Elektronen-Synchrotron DESY, Germany STUDY OF HYBRID SYSTEMS COMPRISING METALLIC NANOPARTICLES, SELF-ASSEMBLED WITHIN ORGANIC MOLECULAR MATRIX O.V. Molodtsova, I.M. Aristova, S.V. Babenkov and V.Y. Aristov</p>	
12.50-13.10		<p>13.00-13.20 DSL119 <u>Dr. Sara Faiz Hanna Tasfy</u> American University of Ras Al Khaimah, United Arab Emirates EFFECT OF CATALYST SYNTHESIS PARAMETERS ON THE PERFORMANCE OF CO₂ HYDROGENATION TO METHANOL OVER SBA-15 SUPPORTED Cu/ZnO-BASED CATALYSTS</p>	