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**Short-lived radicals of purine bases in aqueous solution: reactivity and characterization by magnetic resonance** — ●ALEXEY KIRYUTIN<sup>1,2</sup>, OLGA MOROZOVA<sup>2</sup>, ALEXANDRA YURKOVSKAYA<sup>2</sup>, and HANS-MARTIN VIETH<sup>1</sup> — <sup>1</sup>Department of Physics, Free University of Berlin, D-14195 Berlin, Germany — <sup>2</sup>International Tomography Center of SB RAS, 630090, Institutskaya 3a, Novosibirsk, Russia

The structure of nucleic acids and the mobility of their bases can be probed by the effects of dynamic nuclear spin polarization (CIDNP) created in reversible photoreactions between individual bases and suitable organic dye molecules. For quantitative studies detailed information on the reactions of the dye with the basic building blocks is required. The quenching of triplet excited 2,2'-dipyridyl by the two purine nucleotides guanosine and adenosine monophosphate (GMP and AMP) and the subsequent radical pair decay is a prototype of such a reaction. Laser flash photolysis and CIDNP techniques were applied to get information on the quenching rates and the mechanism of this chemical process and on the structure of the radicals so formed as a function of the pH of aqueous solution. By time-resolved CIDNP the influence of the secondary process of degenerate electron exchange between AMP and its cation radical was studied. For GMP and AMP the CIDNP was measured at variable magnetic field (0..7 T). From simulation of these field dependencies the hyperfine couplings and g-factors of the short-lived neutral, anionic and cationic forms of the nucleoside radicals were determined.

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**Structure and Magnetic Resonance Parameters of the Cationic Radicals of Methionine as Studied by the CIDNP Magnetic Field Dependence** — ●SERGEY KORCHAK<sup>1,2</sup>, KONSTANTIN IVANOV<sup>2</sup>, ALEXANDRA YURKOVSKAYA<sup>2</sup>, and HANS-MARTIN VIETH<sup>1</sup> — <sup>1</sup>Department of Physics, Free University of Berlin, D-14195 Berlin, Germany — <sup>2</sup>International Tomography Center of SB RAS, 630090, Institutskaya 3a, Novosibirsk, Russia

Radical intermediates as they play a key role in many photoreactions often elude spectroscopic characterization because of their high reactivity resulting in a lifetime too short for direct observation. An indirect method exploiting the dynamic spin polarization created in the paramagnetic reaction stage and conserved in the diamagnetic reaction product circumvents this problem. Such a Chemically Induced Dynamic Nuclear Polarization (CIDNP) formed in the reactions of methionine (Met) and N-acetylmethionine (NMet) with triplet excited 4-carboxybenzophenone (CBP) was measured in an external magnetic field of 0-7 Tesla in neutral and basic aqueous solution. The results show that at a pH above 9, the Met cation radical exists in a cyclic form with a two-center three-electron bond between the nitrogen and sulfur atoms, whilst at pH below 9 the Met cation radical has a linear structure. Cation radicals of NMet are formed in linear structure only. By comparing the experimental results with model calculations the g-factors and the hyperfine constants of the cyclic and linear cation radicals were determined. Experimental method and simulation technique will be discussed.

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**Theoretical investigation of the reactivity of Mg deposited on PTCDA films** — ●L. MANCERA, R. SCHOLZ, A. ABBASI, M. SCHREIBER, B.A. PAEZ, G. GAVRILA, G. SALVAN, and D.R.T. ZAHN — Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

In this work, the spectroscopic changes observed upon deposition of Mg on PTCDA films of 15 nm thickness are investigated with different microscopic models for Mg-PTCDA compounds. The Raman spectra obtained on these films reveal pronounced changes of the vibrational fingerprint, indicating the reactive nature of the PTCDA/Mg interface. Some of the new modes observed after Mg deposition can be assigned to modified molecules with magnesium atoms attached to the oxygen atoms in the carboxylic and anhydride groups. In a geometry resembling crystalline PTCDA, the energetically most favourable position for a single Mg atom was found in a bridge position between the oxygen end groups of two adjacent PTCDA molecules. The shift of the 2p core levels of the Mg atoms observed in photoemission spectroscopy results from a significant positive net charge on the Mg atoms, in keeping with the Mulliken charge and core level shift found in the calculation. Due to the delocalized nature of the lowest unoccupied states of neutral PTCDA, the additional negative charge is distributed over the entire molecular area, resulting in relatively small shifts of the O<sub>1s</sub> and C<sub>1s</sub> core levels.

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**Surface properties and haptic perception of soft surfaces** — ●DENYS ZIMIN<sup>1</sup>, KRISTIN SCHMIDT<sup>1</sup>, MEIK RANFT<sup>2</sup>, MARGIT HARSCH<sup>3</sup>, JAN SANDLER<sup>3</sup>, VOLKER ALTSTÄDT<sup>3</sup>, and GEORG KRAUSCH<sup>1</sup> — <sup>1</sup>Physikalische Chemie II, Universität Bayreuth, Universitätsstrasse 30, 95447 Bayreuth, Germany — <sup>2</sup>BASF AG, 67056 Ludwigshafen, Germany — <sup>3</sup>Polymere Werkstoffe, Universität Bayreuth, Universitätsstrasse 30, 95447 Bayreuth, Germany

We study the physical properties of various polymer and leather surfaces (roughness, hydrophobicity, deformability, elasticity and morphology), aiming towards an objective measure of haptic perception of these surfaces by test persons. The surfaces are characterized by subjective evaluations (smooth/rough, waxy, sticky, pleasant/unpleasant, dry, etc.). Correlations between the subjective evaluations and the physical properties are discussed.

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**SFM as a Model System for Local Impact** — ●ALEXANDER GIGLER<sup>1</sup>, SABINE HILD<sup>1</sup>, STEFAN WALHEIM<sup>2</sup>, OTHMAR MARTI<sup>1</sup>, and THOMAS SCHIMMEL<sup>2</sup> — <sup>1</sup>Experimental Physics, University of Ulm, D-89069 Ulm — <sup>2</sup>Institute for Nanotechnology, Forschungszentrum-Karlsruhe GmbH, D-76021 Karlsruhe

For surface characterization using Scanning Force Microscopy (SFM) the understanding of tip-sample interactions is a crucial point. Normal and lateral forces act during such experiments and have to be investigated at the same time to find out the correlations between them. To model these forces a method called Dynamic Friction Force Microscopy (DFFM) has been added to an existing Digital Pulsed Force Mode (DPFM). The crash of a head of a hard-disk into the disk is an example for such an impact. Since this event happens at high speeds (meters per second), the setup has been extended to this range of relative tip-sample velocity.

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**Organically doped sol-gel materials for applications in photodynamic therapy and optical sensing** — ●HALINA PODBIELSKA<sup>1,2</sup>, AGNIESZKA ULATOWSKA-JARZA<sup>1,3</sup>, UWE BINDIG<sup>3</sup>, HANSJ. EICHLER<sup>2,3</sup>, and GERHARD MÜLLER<sup>4</sup> — <sup>1</sup>Bio-Optics Group, Institute of Physics, Wrocław University of Technology, Wybrzeże Wyspińskiego 27, PL-50370 Wrocław, Poland — <sup>2</sup>Institute of Optics, Technical University Berlin, Strasse des 17 Juni 135, D-10623 Berlin, Germany — <sup>3</sup>Laser-und Medizin-Technologie Berlin, Fabeckstr. 60-62, D-14195 Berlin, Germany — <sup>4</sup>Charité Universitätsmedizin Berlin, Campus Benjamin Franklin, Institut für Medizinische Physik und Lasermedizin, Fabeckstr. 60-62, D-14195 Berlin, Germany

The optical properties of photosensitive dyes as may be used for photodynamic therapy or for sensing, entrapped in silica sol-gels, are examined. Our idea is to construct a fiberoptic light applicator which can act as a carrier for photosensitizers. Two photoagents were examined: protoporphyrine PP IX and chlorophyll based Photolon, immobilized in sol-gel coatings on optical fibers. Absorption and emission spectra were measured in air and various environments. It was shown that the dyes preserve their chemical activity, do not leave sol-gel pores, and may contact with even large molecules from external environment. Additionally, we observed that photosensitizers entrapped in sol-gel coatings are sensitive to hydrogen ions, so thus they can be used for pH sensing.

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**Holographische Untersuchungen an azobenzolhaltigen Blockcopolymeren** — ●MICHAEL HÄCKEL<sup>1</sup>, LOTHAR KADOR<sup>1</sup>, CARSTEN FRENZ<sup>2</sup> und HANS-WERNER SCHMIDT<sup>2</sup> — <sup>1</sup>Physikalisches Institut und BIMF, Universität Bayreuth, 95440 Bayreuth — <sup>2</sup>Makromolekulare Chemie I und BIMF, Universität Bayreuth, 95440 Bayreuth

Verschiedene Diblock-Copolymere, die in ihren Seitenketten Azobenzol-Chromophore und zum Teil zusätzlich mesogene Gruppen enthalten, wurden auf ihre Eignung als Medium für volumenholographische Datenspeicher untersucht. Die in einem holographischen Gitter auf Grund der Chromophororientierung erreichbare Brechungsindexmodulation sowie die Stabilität der eingeschriebenen Gitter wurden in Abhängigkeit verschiedener Parameter gemessen. In Proben mit einer Dicke von 1 mm wurde das Verhalten beim Einschreiben mehrerer Gitter unter verschiedenen Winkeln ("Winkel-Multiplexing") untersucht. An der selben Stelle der Probe konnten bis zu 200 Gitter eingeschrieben und eindeutig ausgelesen werden.