CPP 8: POSTERS Dynamics and Diffusion

Time: Monday 16:45–19:00 $\qquad$ Location: Poster A

CPP 8.1 Mon 16:45 Poster A

dynamical and structural properties of sugar surfactant based bicontinuous microemulsions — •Stefan Wellert[1], Matthias Karg[1], Thomas Hellweg[1], Olaf Holderer[2], Hans-Juergen Altmann[3], and Andre Richardt[3] — [1]University Bayreuth, PC I, Universitaetsstrasse 30, D-95440 Bayreuth — [2]Juelich Centre for Neutron Science (JCNS), FZ. Juelich GmbH, Aussenstelle am FRM II, Lichtenbergstr. 1, D-85747 Garching — [3]Bundeswehr Scientific Institute (NBC-Protection), Humboldtstr., D-29633 Munster

Structural and dynamical properties of bicontiuous microemulsions developped for decontamination applications were studied by different scattering techniques. Microemulsion phases with a large internal surface like the bicontinuous region are of main interest for the application as soft and environmental compatible decontamination media for a variety of toxic compounds like pesticides or chemical warfare agents.

Based on APGs, RME, water and an additional alcohol we characterize the phase behavior of such systems as well as the microstructure, investigated using small angle neutron scattering (SANS), neutron spin echo spectroscopy (NSE) and dynamic light scattering.

Additionally, neutron spin echo measurements allow to gain insight into the dynamics of these films and to compare the data with theoretical descriptions like the approach of Zilman and Granek. Beside the undulations of the amphiphilic film also additional contributions due to collective motions are discussed.

CPP 8.2 Mon 16:45 Poster A

Raman spectroscopy of poly- and single-crystalline $12CaO \cdot 7Al_2O_3$ (C12A7) at different temperatures — •Artur S. Seifert[1], Ilia Valov[2], Stefan G. Ebbinghaus[3], Peter J. Klar[1], and Juergen Janek[2] — [1]Institute of Experimental Physics I, Justus-Liebig-University, Heinrich-Buff-Ring 16, D-35392 Giessen. — [2]Institute of Physical Chemistry, Justus-Liebig-University, Heinrich-Buff-Ring 58, D-35392 Giessen. — [3]Solid State Chemistry, University of Augsburg, Universitätsstraße 1, D-86159 Augsburg.

Poly-crystalline $12CaO \cdot 7Al_2O_3$ (mayenite) was synthesized by a solid reaction of Al_2O_3 and $CaCO_3$. Afterwards single-crystalline $12CaO \cdot 7Al_2O_3$ of high purity was produced by a zone melt process. It has been recently suggested that reduced mayenite can be used as transparent conducting oxide (TCO) but this material is also known as an ion conducting solid electrolyte with fast oxygen transport. We study the variation of the vibrational modes of $12CaO \cdot 7Al_2O_3$ as function of temperature in the range from $290\,K$ to $900\,K$ in different atmospheres, i.e. nitrogen, air and water. The vibration properties will be discussed with respect to ion storage and ion mobility within the material.

CPP 8.3 Mon 16:45 Poster A

Rectification in conical nanopores: a one-dimensional Poisson-Nernst-Planck modeling — •Ilona Kosinska[1,2], Igor Goychuk[1], Marcin Kostur[1], Gerhard Schmid[1], and Peter Hanggi[1] — [1]Institut fur Physik, Augsburg, Germany — [2]M. Smoluchowski Institute of Physics, Krakow, Poland

The ion current rectification is studied within a reduced 1D Poisson-Nernst-Planck (PNP) model of synthetic nanopores. A conical channel of a few nm to a few hundred of nm in diameter, and of few μm long is considered in the limit where the channel length exceeds much the Debye screening length. The rigid channel wall is assumed to be weakly charged. A one-dimensional reduction of the three-dimensional problem in terms of corresponding entropic effects is put forward.

The ion transport is described by the non-equilibrium steady-state solution of the 1D Poisson-Nernst-Planck system within a singular perturbation treatment. The analytic formula for the approximate rectification current in the lowest order perturbation theory is given.

The crucial importance of the asymmetry in the potential jumps at the pore ends on the rectification effect is demonstrated. This so constructed 1D theory is shown to describe well the experimental data in the regime of small-to-moderate electric currents.

CPP 8.4 Mon 16:45 Poster A

Diffusion of liquid medium-chain molecules investigated by QENS and PFG-NMR — •Christoph Smuda[1], Gerd Gemmecker[2], Sebastian Busch[1], and Tobias Unruh[1] —

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For the understanding of the functionality of colloidal drug delivery systems the molecule diffusibility inside the colloidal particles is an important parameter. In this contribution it is demonstrated that QENS is well suited for corresponding investigations. However, from measurements of the self-diffusion coefficients of the oligoisoprene derivative coenzyme Q_{10} in nanosized droplets and in the bulk, respectively, at the time-of-flight spectrometer TOFTOF discrepancies to diffusion constants determined by PFG-NMR of more than one order of magnitude have been found. In order to find the origin of these deviations a systematical QENS study with a series of different medium chain n-alkanes was initiated. In accordance to the investigations on Q_{10} it was found that in liquids of medium-chain molecules the diffusion mechanism changes on a nm length scale from a fast short range diffusion to a slower long range diffusion.

[1] T. Unruh, C. Smuda, G. Gemmecker, H. Bunjes, in Quasi-Elastic Neutron Scattering Conference 2006 (QENS2006), P.E. Sokol et al. (Eds.), Mater. Res. Soc. (2007) p. 137

CPP 8.5 Mon 16:45 Poster A

NMR surprizes with thin slices and strong gradients — •Achim Gädke[1], Benjamin Kresse[1], and Nikolaus Nestle[2] — [1]Institute of Condensed Matter Physics, Technische Universität Darmstadt — [2]present address: BASF AG Ludwigshafen GKP/P, G201

In the context of our work on diffusion-relaxation-coupling [1] in thin excited slices, we perform NMR experiments in static magnetic field gradients up to 200 T/m [2]. For slice thicknesses in the range of 10 μm, the frequency bandwidth of the excited slices becomes sufficiently narrow that free induction decays (FIDs) become observable despite the presence of the strong static gradient. The observed FIDs were also simulated using standard methods from MRI physics [3]. Possible effects of diffusion during the FID duration are still minor at this slice thickness in water but might become dominant for smaller slices or more diffusive media. Furthermore, the detailed excitation structure of the RF pulses was studied in profiling experiments over the edge of a plane liquid cell. Side lobe effects to the slices will be disucssed along with approaches to control them. The spatial resultion achieved in the profiling experiments furthermore allows the identification of thermal expansion phenomena in the NMR magnet. Measures to reduce the temperature drift problems are presented.
[1] A. Gädke, N. Nestle 2005 Diffusion Fundamentals 3 38.1-38.12
[2] I. Chang, F. Fujara, B. Geil, G. Hinze, H. Sillescu, A. Tölle, J. Non-Cryst. Sol. 172-174, (1994) 674-681
[3] T. H. Jochimsen, A. Schäfer, R. Bammer, M. E. Moseley, J. Mag. Res. 180 (2006), 29-38

CPP 8.6 Mon 16:45 Poster A

The short time self diffusion coefficient of a sphere in a suspension of rigid rods — •Jan Guzowski[1], Bogdan Cichocki[2], Eligiusz Wajnryb[2], and Gustavo Abade[2] — [1]Max Planck Institute fo Metals Research, Stuttgart — [2]Warsaw University

The short–time self diffusion coefficient of a sphere in a suspension of rigid rods is calculated in first order in the rod volume fraction ϕ. For low rod concentrations the correction to the Einstein diffusion constant of the sphere due to the presence of rods is a linear function of ϕ with the slope α proportional to the equilibrium averaged mobility diminution trace of the sphere interacting with a single freely translating and rotating rod. The two–body hydrodynamic interactions are calculated using the so–called bead model in which the rod of aspect ratio p is replaced by a stiff linear chain of touching spheres. The interactions between spheres are calculated using the multipole method with the accuracy controlled by a multipole truncation order and limited only by the computational power. A remarkable accuracy is obtained already for the lowest truncation order, which enables calculations for very long rods, up to $p=1000$. Additionally, the bead model is checked by filling the rod with smaller spheres. This procedure shows that for longer rods the basic model provides reasonable results varying less than 5% from the model with filling. An analytical expression for α as a function of p is derived in the limit of very long rods. The higher order corrections depending on the

applied model are computed numerically. An approximate expression is provided, valid for a wide range of aspect ratios.

CPP 8.7   Mon 16:45   Poster A

Deuteron NMR studies on ice II — •FLORIAN LÖW[1], MARCO SCHEUERMANN[1], BURKHARD GEIL[2], and FRANZ FUJARA[1] — [1]Institut für Festkörperphysik, TU Darmstadt, 64289 Darmstadt — [2]Experimentelle Physik III, TU Dortmund, 44221 Dortmund

Deuteron spin-lattice relaxation in high pressure ice II has been investigated at different temperatures.

Ice II, one of the high pressure polymorphs of ice, is a completely proton-ordered structure in which two crystallographicly distinguishable types of water molecules form a tetrahedrally linked network of hydrogen bonds.

Deuteron spin-lattice relaxation is sensitive to dynamics in the domain of the Larmor frequency at 46.7 MHz. Measurements at different temperatures of the deuteron spin-lattice relaxation time T_1 show that the magnetization recovery is unequivocally non-exponential which indicates a distribution of correlation times.

The samples (D_2O) have been prepared at appropriate pressures and temperatures. They can be recovered to ambient pressure at liquid nitrogen temperature where they remain metastable and can be studied. The sample quality is verified by x–ray diffraction. T_1–measurements have been performed while increasing the temperature stepwise. At a defined temperature a discontinuity in T_1 indicates a phase transition. The high pressure ice phase transforms to crystalline cubic ice I_c.

CPP 8.8   Mon 16:45   Poster A

Simulation of 3-Pulse Photon Echo with finite pulses — WICHARD BEENKEN and •INES MYNTTINEN — Technische Universität Ilmenau, Fachgebiet Theoretische Physik I

We performed computational simulations of the three-pulse photon echo experiments on Nile-blue as a reference. Our aim is to go beyond the impulsive limit and simulate the effect of a finite duration of the incoming laser pulses. As a first result we could show that the peak shift, i.e. the value of the first delay time where the photon echo is maximum, does not depend linearly on the pulse duration. This complicates the extrapolation of the peak shift to the impulsive limit, where it should theoretically resemble the two-point time correlation function for the fluctuating optical gap M(t). We will show how and up to which degree of time resolution from three-pulse photon echo experiment with finite pulse duration the correlation function M(t), which reflects the dissipative dynamics of the molecule in its environment, can be achieved by computational simulations of the signal dependence on the delay times. Furthermore we will discuss the sophisticated interplay between the intrinsic inhomogeneity of the molecule ensemble and the Fourier-limited spectral width of the incoming laser pulses in three-pulse photon echo experiments.

CPP 8.9   Mon 16:45   Poster A

Phase diagram of octylcyanobiphenyl confined to molecular sieves with hexagonal pore structure — LIGIA FRUNZA[1], STEFAN FRUNZA[1], HENDRIK KOSSLICK[2], and •ANDREAS SCHÖNHALS[3] — [1]National Institute of Materials Physics, R-077125 Magurele, Romania — [2]Leibniz Institute for Catalysis at the University of Rostock, D-18059 Rostock, Germany — [3]Federal Institute for Materials Research and Testing (BAM), 12205 Berlin, Germany

The molecular dynamics of octylcyanobiphenyl (8CB) confined inside the pores of a series of AlMCM-41 samples with long range ordered structure, constant composition (Si/Al=14) but different pore sizes (between 2.3 and 4.6 nm diameter) was investigated by broadband dielectric spectroscopy (10 mHz to 1 GHz) in a large temperature interval. The filed molecular sieves show two relaxation processes: one has a bulk-like behavior and is due to the 8CB molecules in the pore centers. The second relaxation process is due to the dynamics of the molecules in a surface layer. The corresponding relaxation time is ca. two decades slower than that of the first one. Its temperature dependence obeys the Vogel/Fulcher/Tammann (VFT) characteristic for glassy dynamics. The characteristic parameters were obtained by the fit of the VFT-equation to the data and discussed as a function of pore diameter. It was found that the Vogel temperature decreases with increasing pore size.

CPP 8.10   Mon 16:45   Poster A

Gastdynamik im Tetrahydrofuran-Hydrat-Clathrat mit Hilfe der ^2H-NMR — •ANDRE NOWACZYK, BURKHARD GEIL und ROLAND BÖHMER — Experimentelle Physik III, Universität Dortmund, 44221

Dortmund, Germany

Ziel unserer Arbeit ist die experimentelle Untersuchung der Gast-Dynamik in verschiedenen Clathrat-Systemen mit Hilfe der ^2H-NMR. Vorgestellt werden unsere bisherigen Ergebnisse bei der Untersuchung der Gastdynamik in einem Tetrahydrofuran-Hydrat-Clathrat. In diesem System findet ein Übergang von einer breiten, gaußartigen Linie bei Temperaturen über 40 K zu einem statischen Pake-Spektrum bei T¡15 K statt. Dieses Temperaturverhalten ist untypisch und wurde von uns mit Relaxationszeitmessungen untersucht, bei denen wir eine biexponentielle longitudinale Relaxation gefunden haben. Außerdem haben wir neben vollrelaxierten Festkörperechospektren in Abhängigkeit von Temperatur und Pulsabstand auch teilrelaxierte Spektren aufgenommen. Zusätzlich verwenden wir Messungen von Zwei- bzw. Vier-Zeit-Autokorrelationsfunktionen, um die Geometrie der molekularen Gastbewegung und eventuelle dynamische Heterogenitäten genauer zu untersuchen. Der untersuchte Temperaturbereich liegt zwischen 15 K und 45 K. Dort liegt die Dynamik in dem Zeitfenster, das mit unseren experimentellen Methoden zugänglich ist. Wir vergleichen unsere experimentellen Ergebnisse mit Simulationen verschiedener vorgegebener Bewegung.

CPP 8.11   Mon 16:45   Poster A

On the acoustic director interaction in the smectic A phase — •JOSEFINA PERLO[1], LUIS AGUIRRE[1], JORGE REVELLI[2], and ESTEBAN ANOARDO[1] — [1]Universidad Nacional de Cordoba (FaMAF), Cordoba, Argentina — [2]Instituto de Fisica de Cantabria, Santander, Spain

It was shown that an acoustic field can be coupled to the collective dynamics of nematic and smectic-A specimens. Effects of ultrasound on the collective dynamics (order director fluctuations ODF) were observed through the study of the Larmour frequency dispersion of the spin-lattice nuclear magnetic relaxation time.

A fundamental task for the interpretation of the results was the understanding of the interaction mechanism between the acoustic field (a wave vector) and the mesophase director. First works on nematic showed that the acoustic field has an orienting action on the nematic director field.

The idea was extended to the smectic-A phase. The smectic nature of the problem was firstly simplified by considering a nematic in the limit of large anisotropy in the elastic constants. In this limit, the predicted behavior of the relaxation dispersion under sonication showed to be inconsistent. An improved result was obtained by considering the coupling between the smectic order and the ODF.

In this work we investigate details of the interaction between acoustic field and smectic-A phase through the inclusion of elemental features of this phase. We show that the acoustic director interaction can be enhanced if the external acoustic field matches an eigenmode of the smectic system.

CPP 8.12   Mon 16:45   Poster A

Moelcular dynamics in 2D confinement — •CIPRIAN IACOB, ANATOLI SERGHEI, RUSTEM VALIULLIN, ALEXEY KHOKHLOV, JÖRG KÄRGER, and FRIEDRICH KREMER — Institute for Experimental Physics I, University of Leipzig, Leipzig, Germany

Broadband dielectric spectroscopy is employed to study the dynamic glass transition of several glass-forming liquids confined to nanoporous materials with pore sizes smaller than 10 nm. The nanopores are nonintersecting host systems which are prepared by electrochemical anodic etching of a highly doped p-type <100> oriented silicon substrate. The impact of interfacial interaction on the molecular dynamics in 2D confinement is analysed as well by coating the inner surface of the pores with different anorganic or organic surfactants.

CPP 8.13   Mon 16:45   Poster A

TD-NMR studies on CuSO4 salt hydrates — •NIKOLAUS NESTLE[1], SEBASTIAN KLEINSCHMIDT[2], PETER MAGIN[1], and ROBERT WENGELER[1] — [1]BASF Aktiengesellschaft, Ludwigshafen — [2]Universität Magdeburg, FB Chemie

Despite the high concentration of paramagnetic copper ions, solid CuSO4 hydrates exhibit surprizingly narrow NMR signals. This is known since the late 1940s [1]. Using TD-NMR methods established for polymer studies, the relaxation behaviour of CuSO4 preparations with different water content was studied at room temperature. For the water content of the pentahydrate and below, the NMR signal exhibits a pure solid-state-type magnetization decay behaviour. For slightly overstoichiometric moisture contents, a liquid-like signal is observed in addition to the solid signal. However, the relative amplitudes

of the solid and the liquid signal do not mirror the stoichiometric composition of the pentahydrate and the excess water. Instead, the solid signal amplitude only accounts for four hydrate water molecules while the fifth water exhibits rapid exchange with the liquid phase and thus contributes to the liquid-type signal. This finding is in good agreement to results from investigations into the crystal structure of solid CuSO4 pentahydrate [2].

[1] N. Bloembergen, Physica 16, 95-112 (1950). [2] J.J. Rush, J.R. Ferraro, A. Walker, Inorganic Chemistry 6, 346-351 (1967).

CPP 8.14   Mon 16:45   Poster A

Adsorption Kinetics of Individual Dye Molecules on Semiconductor Nanocrystal Surfaces — •Mario Heidernätsch[1], Thomas Blaudeck[1,2], Jörg Schuster[1], and Christian von Borczyskowski[1] — [1]Optical Spectroscopy and Molecular Physics, TU Chemnitz, 09107 Chemnitz, Germany — [2]Print and Media Technology, TU Chemnitz, 09107 Chemnitz, Germany

Grafting of colloidal semiconductor quantum dots (QDs) with organic molecules is a common approach to adjust their optical, chemical, and electronic properties. In this respect, QD surfaces offer a certain yet finite number of binding sites to functionalization with molecules. With that, however, the common concepts of bimolecular reaction kinetics including their dissociation constants do not hold any more.

In our computational study, we employ numerical ab-initio techniques to separate the nanoaggregate formation process into the Brownian motion of an individual molecule in solution and its eventual adsorption and desorption in the potential of a particular binding site on the QD surface. Interestingly, the extrapolation of these elementary processes to an ensemble of QDs and molecules allows insights into the relationship between surface coverage and binding energies. Conclusions thereon are up to date impossible to draw solely by experimental methods. The comparison with previous results on the formation kinetics further backs the presence of a dynamic equilibrium.

CPP 8.15   Mon 16:45   Poster A

viscosity and structural alteration of a coarse-grained model of polystyrene under steady shear low studied by reverse nonequilibrium molecular dynamics — •paola carbone, xiaoyu chen, and florian müller-plathe — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, Petersenstrasse20 D-64287 Darmstadt, Germany

The reverse nonequilibrium molecular dynamics (RNEMD) method is implemented to predict the viscosity of a coarse-grained model of short-chain polystyrene. The coarse-grained model has been derived to reproduce the structure of polystyrene. It is therefore not a generic model, but polymer-specific. The zero-shear viscosity from simulation result is linearly dependent on the molecular weight for short-chain systems, in agreement with experiments and the theoretical prediction of the Rouse model. The shear-thinning behaviour for all studied systems follows a power law. The exponent of the power law depends on the chain length and it increases with the molecular weight. The zero-shear viscosity is also compared with experimental data, where the pronounced difference found is originated mainly by the inherent dynamic properties of the coarse-grained model used. The structural changes under shear are quantitatively investigated, indicating that the process of chain alignment, in combination with chain stretching, leads to a macroscopic anisotropy of the material.

References

1.X. Chen, P. Carbone, W. Cavalcanti, G. Milano, F. Müller-Plathe, Macromolecules, 2007, 40, 8087-8095

CPP 8.16   Mon 16:45   Poster A

Soft spots of hard spheres — •Erik Lange — University of Konstanz

The influence of the potential shape on the structure and dynamics of a colloidal suspension has been of longstanding interest. We use simulations to tackle this question from a new angle.

Exploiting molecular dynamics simulations we find strong differences in the local structure for different potentials. Even a rescaling with respect to the distance from the freezing point does not reconcile this disagreement. However the structure factor

$$S_q = \frac{1}{N} \sum_{ij} \exp\left[i(\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j))\right]$$

shows a remarkable indifference towards subtleties in the potential.

The fact that a number of different systems display the same structural property suggests a closer look at the structural relaxation. As a result our work provides a clear tool to predict where differences should be negligible.

Indeed the longtime diffusion coefficients coincide as well as the stress-stress correlation at intermediate to long times.

So this is an approach that makes it clearer where softness matters and where hard spheres have soft spots.

CPP 8.17   Mon 16:45   Poster A

A colloidal approach to unspecific protein adsorption of protein films — •Olaf Leidinger, Markus Bellion, and Ludger Santen — Fachrichtung theoretische Physik, Universität des Saarlandes, 66041 Saarbrücken

We investigate the unspecific adsorption of proteins, which are modelled as colloidal particles. The particle-particle interactions are described in the framework of the DLVO theory, which includes steric repulsion, electrostatic and van der Waals interactions. In addition to this, we introduce an internal degree of freedom representing different conformations of the model protein at the surface.

By means of extensive Monte Carlo simulations we reproduce the experimentally observed characteristics of the biofilm formation. The adsorption kinetics can be divided into three intervals: Initially the adsorption is limited by the flux of particles to the surface. In a second interval one observes domain formation of compactified proteins and finally the surface coverage reaches its stationary value. The robustness of this scenario is scrutinized for various model parameters.

CPP 8.18   Mon 16:45   Poster A

NMR studies of mobility on ferrocene adsorbed in MOF-5 — •Markus Wehring[1], Pieter C. M. M. Magusin[2], Saeed Amirjalayer[3], Rochus Schmidt[3], and Frank Stallmach[1] — [1]Faculty of Physics and Earth Sciences, University of Leipzig, Germany — [2]Chemical Engineering and Chemistry, Eindhoven University of Technology, Netherlands — [3]Faculty of Chemistry and Biochemistry, Ruhr-University Bochum, Germany

Metal-organic frameworks (short: MOF) are a relatively new class of crystalline materials with a nanoporous structure. MOFs consist of metal coordination centres and organic linkers forming a three dimensional pore system with prospective applications in heterogeneous catalysis, separation and gas processing. In this study we investigate the host-guest interaction of MOF-5 ($Zn_4O(bdc)_3$) loaded with ferrocene ($FeC_{10}H_{10}$) via two-dimensional MAS NMR and PFG NMR techniques. In agreement with computer simulations, we found that the adsorbed ferrocene molecules are located close to the carbon rings of the organic linkers of the MOF-5 lattice. Additional the self-diffusion-coefficient were measured and compared with results of MD simulations.

CPP 8.19   Mon 16:45   Poster A

Charging dynamics of carbon nanotube forest electrodes — •Lars Pastewka[1] and Michael Moseler[1,2] — [1]Fraunhofer Institut für Werkstoffmechanik, Wöhlerstraße 11, 79108 Freiburg, Germany — [2]Freiburger Materialforschungszentrum, Stefan-Meier-Straße 21, 79104 Freiburg, Germany

Efficient energy harvesting requires devices which are able to store large amounts of electrical energy in short times. In this context, electrostatic double-layer capacitors with nanostructured electrodes have been discussed. Here, we exemplarily analyse ion transport into carbon nanotube forest electrodes in order to extract response times and capacities using a multiscale modeling approach. Starting from a quantum mechanical treatment of the capacitance of single tubes we construct a molecular dynamics model for ion transport into these electrodes. Finally, a continuum transport equation is derived which reproduces the molecular dynamics results and can be used for investigating systems with realistic forest heights and electrode separations.

CPP 8.20   Mon 16:45   Poster A

Travelling Fronts in an A+B -> 2A Reaction under Subdiffusion — •Daniela Froemberg and Igor M. Sokolov — Humboldt University, Berlin

Using the continuous time random walks approach, we derive the analog of the Fisher-Kolmogorov-Petrovskii-Piskunov equation for subdiffusion, having a form of an integro-differential equation. In contrast to the normal F-KPP equation, the reaction introduces a nonlinearity into the transport term which in addition contains a fractional derivative. We show that the subdiffusive F-KPP equation includes the normal equation as a limiting case. Linearizing the equation in

the leading edge of the traveling front we obtain the velocity of the front and investigate its dependence on the subdiffusion parameter alpha, the generalized diffusion coefficient, and the local reaction rate coefficient.