DF 9: Poster

Time: Tuesday 15:00–18:00 Location: Poster G

DF 9.1 Tue 15:00 Poster G

Tuning the Li diffusivity of poor ionic conductors by mechanical treatment: High Li conductivity of nanocrystalline $LiTaO_3$ — •Viktor Epp, Martin Wilkening, Armin Feldhoff, and Paul Heitjans — Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover, Callinstr. 3-3a, 30167 Hannover

Lithium tantalate, $LiTaO_3$, with an average particle size in the μm range is known as a very poor Li ion conductor. It is shown that its Li conductivity can be drastically increased by ball-milling. The thus obtained nanostructured powder with an average particle size of about 20 nm shows a dc conductivity, σ_{dc}, of about $3 \cdot 10^{-6}$ S cm^{-1} at $T = 450$ K ($\sigma_{dc}T = 1.4 \cdot 10^{-3}$ S cm^{-1} K) which is about five orders of magnitude larger than that of the corresponding microcrystalline powder at the same temperature. The activation energy E_A is reduced by about one third, i. e., it decreases from $E_A = 0.90(1)$ eV to about $E_A = 0.63(1)$ eV. Similar results were previously obtained for lithium niobate [1]. The effect of different milling times on the ionic conductivity is studied. Furthermore, the thermal stability of the nanocrystalline materials against grain growth has been checked by *in situ* impedance spectroscopy. Interestingly, the Li conductivity of a sample milled for 16 h does not change much even when the material is exposed to about 700 K for several hours. Moreover, the Li self-diffusion in the nanostructured as well as the coarse grained materials is elucidated by various solid-state ^{7}Li NMR techniques.

[1] P. Heitjans, M. Masoud, A. Feldhoff, M. Wilkening, *Faraday Discuss.* **134** (2007) 67.

DF 9.2 Tue 15:00 Poster G

Nanoporöse Festkörperfarbstoffhybride — •Jennifer Krause, Andrea Schuy, Theo Woike und Dominik Schaniel — 1.Physikalisches Institut , Universität zu Köln

Farbstofflaser können über einen großen Spektralbereich von ultraviolett bis ins nahes infrarot sowohl im CW-Modus als auch gepulst betrieben werden. Ein Festkörperfarbstoffmaterial hätte gegenüber den bisher in Farbstofflasern verwendeten Flüssigkeiten viele Vorteile. Eine Möglichkeit Festkörperfarbstoffmaterialien zu realisieren ist es die Farbstoffe in eine geeignete Matrix einzubetten. Diese Matrix muss eine hohe optische Qualität haben und in einem weiten Spektralbereich transparent sein. Ebenso soll sie eine hohe Zerstörschwelle gegenüber Laserstrahlung und eine große thermische- und photochemische- Stabilität aufweisen. Geeignete Matrizen die diese Ansprüche erfüllen sind Xerogele [1]. Wir haben Xerogele nach dem Sol-Gel Verfahren [2] hergestellt und sie mit Farbstoffen beladen. Mittels Lumineszenz Spektroskopie untersuchen wir, welchen Einfluss die Konzentration der Farbstoffe in den Gelen und die Porengröße der Gele auf die Lumineszenz Eigenschaften sowie die Lebensdauer der Laserfarbstoffe haben.

[1]E. Yariv, S. Schultheiss, T. Saraidarov, R. Reisfeld, Optical Materials vol.16, p.29 (2001)

[2] N. Hüsing, U. Schubert, Angewandte Chemie Int. Ed. vol. 37, p. 23 (1998)

DF 9.3 Tue 15:00 Poster G

Low-coherence microscopy versus projected fringe method for the study of surface topography of photo inkjet papers — •Kai Brune[1,2], Mirco Imlau[1], and A. Knittel[2] — [1]Department of Physics, University of Osnabrück, D-49069 Osnabrück — [2]Felix Schoeller Service GmbH, Burg Gretesch, D-49086 Osnabrück

We have investigated the topography of photo inkjet paper surfaces in different production steps. The aim of our work was to optimize the paper quality and to find a method for quality assurance. The topography analysis of the surface was performed by low-coherence microscopy and projected fringe method. From the roughness and the surface analysis a correlation between the paper quality and the surface structure was found. The quality of the photo inkjet paper is defined by the quality of the paper surface and the printing characteristics. Both methods for surface analysis were compared and the advantages and disadvantages were discussed. Some basic information is presented on this poster. The studies were performed in cooperation with the Felix Schoeller Service GmbH in Osnabrück.

DF 9.4 Tue 15:00 Poster G

Interface properties of $PbTiO_3$ and PZT thin films on Pt-terminated substrates — •Salah Haboutі[1], Claus-Henning Solterbeck[1], Mohammed Es-Souni[1], Vladimir Zaporojtchenko[2], and Franz Faupel[2] — [1]Institute for Materials and Surface Technology, University of Applied Sciences Kiel — [2]Chair for Multicomponent Materials, Christian-Albrechts-Universtät zu Kiel

Electrical properties of $Pb(Zr_{0.52}Ti_{0.48})O_3$ (PZT) and $PbTiO_3$ thin films are influenced by processes at the interface with the substrate. These interfaces are investigated for sol-gel processed thin films on Pt-terminated substrates. XPS depth profiles from samples prepared at various temperatures and in situ XRD measurements at different temperatures reveal the stochiometry and transformation kinetics at the interfaces. An intermediate phase with Pt and Pb emerges at the beginning of the film formation, but it disappears completely when the crystallization is complete.

DF 9.5 Tue 15:00 Poster G

Transmission of light through subwavelength holes in thin metal films — •Mathieu Gentile[1,2], Felix Kalkum[1], Manfred Fiebig[2], and Karsten Buse[1] — [1]Physikalisches Institut, Wegelerstraße 8, 53115 Bonn, Germany — [2]Helmholtz-Institut für Strahlen- und Kernphysik, Nussallee 14 - 16, 53115 Bonn, Germany

It was discovered a decade ago that a hole array in a thin metal film with hole diameters much smaller than the wavelength, λ, exhibit a transmission efficiency, η, higher than 100% in the visible range. Here, η denotes the intensity of light transmitted through the hole in relation to the intensity incident onto the hole area. Unfortunately, a satisfactory understanding of the intensity enhancement has not been reached up to date. The present work is devoted to the experimental quantification of η for transmission through a single circular hole. In particular, phase-conjugation experiments, in which holograms are recorded in $LiNbO_3$ crystals by focusing light onto a small hole in a metal film, will benefit from this quantification. Thus, $LiNbO_3$ crystals are used as a substrate for a 200-nm-thick gold metal film illuminated by a 532-nm-frequency-doubled Nd:YAG laser. Using the knife-edge method a Gaussian profile with radius of 3.82 μm and total power of 81 mW is determined for the focused beam. A peak transmission efficiency of $(335 \pm 7)\%$ is observed for a 350-nm-diameter hole ($2r/\lambda$=0.66).

DF 9.6 Tue 15:00 Poster G

Formation of nanoporous alumina films in sulphosalicylic acid solution — •Piotr Hamolka[1], Igor Vrublevsky[1], Vitaly Sokol[1], and Liubou Hamolka[2] — [1]Department of Nano- and Microelectronics, BSUIR, Minsk, Republic of Belarus — [2]The Institute of General and Inorganic Chemistry of the NAS of Belarus, Minsk, Republic of Belarus

This work presents the results studying the volume expansion factor of porous alumina films, formed by through anodizing of an aluminum foil of 11.5 μm thickness in a 0.6M sulphosalicylic acid solution. The thickness of porous alumina films was measured by an optical microscopy. The volume expansion factor of nanoporous alumina films in the range of anodizing current densities of 1.0 * 60 mA cm^{-1} varied from 1.23 to 1.64. The obtained results demonstrated linear dependence for the current density logarithm versus the inverse volume expansion factor. The curve on this plot was found to be consisted of two subsequential rectilinear regions. We suggested that the change in the film oxide growth is the evidence of modification of the structure of Helmholtz layer in the sulphosalicylic acid electrolyte with increasing of anodizing current. The structure of oxide films obtained at different anodizing current densities was studied with thermogravimetric analysis.

DF 9.7 Tue 15:00 Poster G

Probing nanoscale ferroelectricity by photoemission - the $PbTiO_3$ / Nb-$SrTiO_3$ (100) system — •Eike F. Schwier[1], Laurent Despont[1], Céline Lichtensteiger[2], Claude Monney[1], Corsin Battaglia[1], Matthew Dawber[2], Gunnar Garnier[1], Jean-Marc Triscone[2], and Philipp Aebi[1] — [1]Institut de Physique, Université de Neuchâtel, CH-2000 Neuchâtel, Switzerland — [2]DPMC, Université de Genève, Switzerland

Ferroelectric thin films have become more and more important as possible substituents of ferromagnetic storage devices. To utilize these new materials within the lowered dimensionality of modern electronics, one has to investigate the limits of the films functionality. Two

questions are especially important. Does a critical thickness for ferroelectricity exist? And what does the interaction of the electrodes with the film change inside the film?

We performed photoemission experiments on ultra thin $PbTiO_3$ films grown on Nb-$SrTiO_3$ (100) in order to probe the properties close to the surface and at the atomic scale. X-ray photoelectron diffraction maps are used to probe the intra-cell polar atomic distortion and tetragonality associated with ferroelectricity at the surface. Thickness and mean detection depth dependencies in X-ray photoelectron spectroscopy data lead to a semi-classical model which might be able to describe the electrostatic potential course across the system. To estimate the influence of sample charging versus the charge displacement created by the ferroelectricity, a time and intensity dependent shift in the photoelectron kinetic energy is exploited.

DF 9.8 Tue 15:00 Poster G

Soft, flexible and conformable ferroelectret touchpad — •Gerda Buchberger, Reinhard Schwödiauer, and Siegfried Bauer — Soft Matter Physics, Johannes Kepler University, Altenbergerstr. 69, 4040 Linz, Austria

Flexible electronics is a driving impetus in plastic electronics. Besides displays, electronic components are required for the communication between the human users and the device, examples include touchpads or touchscreens. To be used in plastic electronics, such elements should be prepared as easy as possible, thereby complex array constructions of sensors are outruled. Here we describe a very simple, soft, flexible and conformable touchpad based on cellular ferroelectrets with a strong longitudinal piezoelectric effect. Thereby the device is insensitive to bending piezoelectricity and only activated by the touch of a user. Instead of array sensors, a large area sensor element is described with electronic components at the periphery. In order to determine the minimum number of electronic elements at the periphery, topological and symmetry arguments are employed. In addition the symmetry breaking of ferroelectrets along the thickness direction of the foil may be used to advantage. We describe a simple single touch input/output device, and present first investigations of the characteristics of the element. Work partially supported by the FWF.

DF 9.9 Tue 15:00 Poster G

Charge transport in composite-materials containing carbon nano-tubes and carbon nano-fibers — •Michael Konter[1], Pablo Carballeira[2], Frank Haupert[2], Bernd Wetzel[2], Alois K. Schlarb[2], and Rolf Pelster[1] — [1]Fachrichtung 7.2 Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany — [2]Institut für Verbundwerkstoffe GmbH, Kaiserslautern, Germany

We have investigated the electric transport properties of composite materials using temperature dependent dielectric spectroscopy (200 Hz - 2 GHz, 70 K - 290 K). The samples consist of epoxy-resin containing up to 2 vol. % carbon nano-tubes and carbon nano-fibers, respectively. The dispersion was achieved with a torus mill and / or a three roll calender device. We observe percolation as well as an associated polarization process. Its characteristic frequency and its dielectric strength are correlated with the dc-conductivity. This behaviour is discussed in terms of the micro-structure.

DF 9.10 Tue 15:00 Poster G

Investigation of the uniaxial relaxor calcium barium niobate by k-space spectroscopy and pyroelectric methods: a comparison to strontium barium niobate. — •Urs Heine[1], Uwe Völker[1], Klaus Betzler[1], Manfred Burianek[2], and Manfred Mühlberg[2] — [1]University of Osnabrück, Department of Physics, Barbarastr. 7, 49076 Osnabrück — [2]University of Cologne, Institute of Crystallography, Zülpicher Str. 49b, 50674 Cologne

The ferroic relaxor strontium barium niobate (SBN) has been considered as a promising material for optical applications, but the low phase transition temperature region prevents reliable utilization of its ferroelectric characteristics. Here, we present comparative investigations of the unfilled tungsten bronze calcium barium niobate (CBN) using k-space spectroscopy and pyroelectric measurements. Contrary to SBN, CBN shows a limited stability region in the range of about 20 and 40 mole fraction calcium. Congruently melting CBN (28.1 mole fraction calcium [1]) shows a relaxor phase transition analog to that in SBN at approximately 540 K, 200 K higher than that of SBN61. By applying external electric fields to CBN, we find similar behaviour as for SBN [2], even though the anisotropy in the distribution of the domain-sizes arises at higher fields. Thus, we conclude that CBN - like SBN - exhibits a domain size dependent ferroelectric characteristic, too.

[1] M. Burianek, B. Joschko, I. Kerkamm, T. Schoenbeck, D. Klimm, M. Muehlberg: J. Crystal Growth 229, 413-417 (2007)

[2] U. Voelker, U. Heine, C. Gödecker, K. Betzler: Journal of Applied Physics: in print (2007)

DF 9.11 Tue 15:00 Poster G

Confocal Raman and Fluorescence Lifetime Imaging (FLIM) Microscope — •Philipp Schreier[1], Lothar Kador[1], Deliani Lovera[2], and Volker Altstädt[2] — [1]University of Bayreuth, Institute of Physics and BIMF, 95440 Bayreuth — [2]University of Bayreuth, Department of Polymer Engineering, 95440 Bayreuth

We present a custom-built set-up capable of performing three-dimensional confocal Raman and fluorescence lifetime imaging (FLIM) microscopy. 3-d Raman measurements were performed on spider silk fibers and electro-spun electret fibers which were prepared from miscible and non-miscible polymer mixtures. In both cases of the electret materials, the compositions of the fibers were homogeneous on the micrometer scale. For the FLIM experiments the cw laser is modulated with an acousto-optic modulator in the MHz regime, and the phase shift of the fluorescence light with respect to the excitation is measured. In this way, fluorescence lifetimes in the nanosecond range can be obtained. First data of, e. g., paper samples stained with different fluorescent dyes are presented.

DF 9.12 Tue 15:00 Poster G

Topographic investigations of LiB_3O_5-crystal surface degradations generated at reduced and normal pressure — Stefan Möller, •Änne Andresen, and Mirco Imlau — Department of Physics, University of Osnabrück, D-49069 Osnabrück

We have investigated the degradation of LiB_3O_5-crystal surfaces during long-term irradiation with intense laser light of $\lambda = 355\,\mathrm{nm}$, $\lambda = 532\,\mathrm{nm}$, or $\lambda = 1064\,\mathrm{nm}$ wavelength, and different repetition rates up to 100 kHz as well as cw-light. The topographic analysis of the surfaces were performed with low-coherence and atomic-force microscopy. At reduced pressure a catastrophic degradation of the surface was already observed upon irradiation with green light, whereas at normal pressure UV-radiation was necessary for the generation of surface degradation. The surface degradation emerge faster upon increase of the light intensity. A model for the generation of the observed surface degradations related to thermal damage will be presented. The general applicability of low-coherence microscopy as a method to analyze light-induced degradations of LiB_3O_5-crystal surfaces is considered. Financial support by the DFG (TFB 13, project A5/13-04).

DF 9.13 Tue 15:00 Poster G

Influence of Mg-doping on the lifetime of optically generated small polarons in $LiNbO_3$ — •Daniela Conradi[1], Bettina Schoke[1], Christoph Merschjann[1], Mirco Imlau[1], Gabor Corradi[2], and Katalin Polgár[2] — [1]Fachbereich Physik, Universität Osnabrück, Osnabrück, Germany — [2]Hungarian Academy of Sciences, Budapest, Hungary

Excitation and recombination of optically generated small electron and hole polarons in Mg-doped $LiNbO_3$ is investigated by means of time-resolved excited-state-absorption (ESA) spectroscopy. Transient light-induced absportion changes $\alpha_{\mathrm{li}}(t)$ are observed in the visible and near infrared spectral range upon excitation with intense green laser pulses ($\lambda = 532\,\mathrm{nm}, \tau = 8\,\mathrm{ns}, I_\mathrm{p} \leq 1400\,\mathrm{GW/m^2}$). The results indicate the generation of bound small O^- hole polarons and bound small Nb_{Li}^{4+} electron polarons in $LiNbO_3$:Mg with doping concentrations below the optical-damage-resistance threshold. In contrast, for concentrations above this threshold the light-induced absorption is caused by hole polarons and free small Nb_{Nb}^{4+} electron polarons. In either case the characteristics of $\alpha_{\mathrm{li}}(t)$ in the blue-green spectral range point to the presence of further extrinsic impurities — most likely $Fe^{2+/3+}$.

We present a model concerning all these types of polarons for $LiNbO_3$ doped with Mg below and above the optical-damage-resistance threshold. The influence of additional extrinsic impurities on the excitation and recombination of the small polarons is discussed.

Supported by the Deutsche Forschungsgemeinschaft (Projects IM 37/2-2 and TFB 13-04).

DF 9.14 Tue 15:00 Poster G

Amplitude-Frequency-Characteristics of Ferroelectric Thin-Films — •Kay Barz, Martin Diestelhorst, and Horst Beige — Martin Luther-Universität Halle-Wittenberg

The dielectric properties of ferroelectric thin films are commonly stud-

ied by means of low-frequency or quasi-static methods (capacitance-voltage, current-voltage, hysteresis). We pursue a different approach by investigating the frequency response of a LCR series-resonant circuit containing a ferroelectric thin film as capacitance. The poster presents amplitude-frequency-characteristics (AFC) observed at different types of thin film samples (Metal/Ferroelectric/Metal and Metal/Ferroelectric/Semiconductor). The differences among them are pointed out and a comparison is made with respect to the typical response of a ferroelectric bulk material.

The results show, how hysteresis and its transient alterations due to fatigue manifest in a shift of resonance frequency. This behaviour can be simulated numerically, and thus explain the observed deviations of the AFC from a linear response.

DF 9.15 Tue 15:00 Poster G

Interfacial ion conduction in nanostructured solid electrolytes measured by Electrostatic force microscopy — •Ahmet Taskiran[1], Andre Schirmeisen[1], Bernhard Roling[2], and Bracht Hartmut[3] — [1]Physikalisches Institut,Wilhelm-Klemm-Str.10,48149 Münster,Germany — [2]Institut für Phys.Chemie,Hans-Meerwein-Str.,35032 Marburg,Germany — [3]Institut für Materialphysik, Wilhelm-Klemm-Str.10,48149 Münster,Germany

Solid ion conductors are applied in super-capacitors, high energy storage batteries and chemical sensors. Recent work has shown an enhancement of the overall conductivity by interfaces between different materials. Since the macros. measurements yield an average value over a large regime, an investigation on nanoscopic scale is needed to understand the ion dynamic. We use electrostatic force microscopy (EFM) operating in the noncontact mode, which use a sharp tip with an apex radius of 10 nm as measuring sensor. Therefore, the investigations of ion transport occur in nanoscopic volume. The investigation of temperature dependent ion conductivity was monitored in the range from 100-675 K, yielding the activation energies of the ion hopping process [1]. We measured the activation energies of nanocrystallites as well as the glass matrix in a partially crystallized LiAlSiO sample, which are in good agreement with macroscopic results [2] and identified an additional activation energy which can be attributed to the ions at the interface between both phases [3].[1]Schirmeisen et al.,Appl. Phys. Lett.85(2004)2053 [2]Roling et al.,Phys.Chem.Chem.Phys.7(2005)1472 [3]Schirmeisen et al.,Phys.Rev.Lett.98(2007)225901

DF 9.16 Tue 15:00 Poster G

First-principles investigation of thin $A\mathbf{TiO_3}$ films with stacking faults — •Kourosh Rahmanizadeh, Gustav Bihlmayer, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

The ferroelectric polarization is a fundamental quantity which is used for the realization of nanoelectronic devices applicable in information technology. Experimental studies have shown that defects and stacking faults play an important role in ferroelectric materials. Employing density functional theory calculations based on the full-potential linearized augmented planewave (FLAPW) method as realized in the FLEUR code (www.flapw.de), we study the polarization of thin films of the perovskite $ATiO_3$ compounds $PbTiO_3$ and $BaTiO_3$. Both AO-terminated and TiO_2-terminated surfaces with the polarization in the film plane or perpendicular to the surface are considered. We present studies on the applicability of different exchange-correlation potentials and first results on the influence of stacking faults at the surfaces on the ferroelectric polarization in these compounds.

DF 9.17 Tue 15:00 Poster G

Antiferroelectric / ferroelectric $\mathbf{PbZrO_3}$ / $\mathbf{Pb(Zr_{0.8}Ti_{0.2})O_3}$ multilayers: properties and effects — •Ksenia Boldyreva[1], Lucian Pintilie[1,2], Andriy Lotnyk[1], Nikolai Zakharov[1], Marin Alexe[1], and Dietrich Hesse[1] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle/Saale, Germany — [2]NIMP, P.O. Box MG-7, 077125 Bucharest-Magurele, Romania

Epitaxial antiferroelectric / ferroelectric $PbZrO_3$ / $PbZr_{0.8}Ti_{0.2}O_3$ (PZO/PZT) multilayers (MLs) were grown by pulsed laser deposition on $SrTiO_3$(100) substrates, covered with a $SrRuO_3$ (100) bottom electrode and a thin tetragonal $PbZr_{0.2}Ti_{0.8}O_3$ buffer layer. Hysteresis, switching current-voltage and capacitance-voltage curves of the MLs with an individual layer thickness above 10 nm show a mixed AFE-FE behavior, whereas below 10 nm the MLs show only FE behavior. Obviously the $PbZrO_3$ layers thinner than 10 nm underwent a transition into the ferroelectric state with a corresponding symmetry change from orthorhombic to rhombohedral. An X-ray diffraction ϑ-2ϑ scan and Reciprocal Space Mapping showed a corresponding orthorhombic-to-rhombohedral transition of the $PbZrO_3$ layers [1]. High-resolution TEM images were taken in order to investigate the microstructure of the PZO/PZT multilayers. The observations are discussed in terms of a strain effect.

[1] K. Boldyreva, L. Pintilie, A. Lotnyk, I. B. Misirlioglu, M. Alexe, and D. Hesse, Appl. Phys. Lett. **91**, 122915 (2007)

DF 9.18 Tue 15:00 Poster G

Effects of $\mathbf{MoO_3}$ and $\mathbf{WO_3}$ on phase separation of a soda-lime-silica glass — •Rainer Kranold[1] and Armin Hoell[2] — [1]Institut für Physik, Universität Rostock, D-18051 Rostock, Germany — [2]Hahn-Meitner-Institut Berlin, D-14109 Berlin, Germany

The base glass, $13Na_2O$-$11CaO$-$76SiO_2$, undergoes subliquidus phase separation. Below the binodal temperature, T_b, the glass separates into two amorphous phases, silica enriched droplets and a silica-poor matrix. The phase separation process is governed by two competitive parameters, the thermodynamic driving force, $\Delta\mu$, and the interface tension, σ. Here, the effects of small MoO_3 and WO_3 additions to the base glass on the parameters $\Delta\mu$ and σ are investigated. By determination of the wetting angle of a drop of the liquid glass melt on the flat surface of pure silica glass it was found that additions of MoO_3 or WO_3 to the base glass increase the value of σ. The growth process of the droplets at 600 °C in glasses with and without MoO_3 or WO_3 was studied by small-angle X-ray scattering (SAXS). All of the glass samples were in the early stage of diffusion controlled coarsening. However, while in the pure glass the volume fraction, w, of the droplets continuously approaches its reported equilibrium value, w_e, the w values of the doped glasses exceed considerably the value of w_e. These findings can be explained by the assumption that the additives MoO_3 and WO_3 give rise to an increase of $\Delta\mu$ resulting in a shift of the miscibility gap to higher temperatures. By means of in situ high-temperature SAXS experiments, it was proved that T_b of the doped glasses is really increased in relation to that of the base glass.

DF 9.19 Tue 15:00 Poster G

Polarisationseffekte in dielektrischen Substraten — •bernhard faber — Institut für theoretische Physik 2, Uni. Erlangen, Deutschland

Durch Metallcluster ausgelöste Polarisationseffekte in dielektrischen Substraten werden behandelt. Untersucht werden Na_N-Cluster ($N < 10$) auf Cu(111) bzw. auf Ar-Schichten, die wiederum auf Cu(111) abgelegt werden.

Die Beschreibung des Clusters und der Oberfläche erfolgt in einem hierarchischen TD-DFT-MD-Modell. Die Valenzelektronen der Na-Atome werden mittels TD-LDA behandelt. Die Ankopplung der Na^+-Ionen und des Ar-Substrats erfolgt mit Hilfe lokaler Pseudopotentiale. Die Polarisationswechselwirkung des Cu-Substrats mit dem Na- und Ar-Adsorbat wird durch Bildladungen vermittelt.

Wir berechnen Schnitte durch die Born-Oppenheimer-Flächen. Im Fall zwischenliegender Ar-Layer werden Druckeffekte auf das Argon beobachtet. Ohne Pufferung ergibt sich ein Transfer von Elektronendichte ins Metall, und damit eine starke Polarisierung des Clusters.