

# LABORATORY OF THEORETICAL PHYSICS AND COMPUTER MODELLING

Head of Laboratory Dr. hab. phys. Eugene Kotomin

## Research Area and Main Problems

Our theoretical research interests are focused on five classes of problems related to:

- kinetics of diffusion-controlled processes, with emphasis on pattern formation and catalytic surface reactions;
- the atomic and electronic structure of numerous advanced materials, with emphasis on calculations of properties of defects, surfaces, metal/insulator interfaces.
- theoretical simulations and experimental studies of nanostructures and nanomaterials;
- stochastization of magnetic field lines in magnetized fusion plasma;
- gyrotron development for thermonuclear reactors .

We combine several different techniques, including analytical formalisms and large-scale computer simulations (quantum chemical methods, stochastic simulations as well as Monte Carlo/cellular automata modeling).

## Scientific staff

1. Dr. hab. E. Kotomin
2. Dr. hab. V. Kuzovkov
3. Dr. O. Dumbrajs
4. Dr. R. Eglitis
5. Dr. D. Gryaznov
6. Dr. V. Kashcheyevs
7. Dr. Yu. Mastrikov
8. Dr. S. Piskunov
9. Dr. A. Popov
10. Dr. Yu. Zhukovskii
11. Dr. G. Zvejnieks

## PhD students

12. D. Bocharov
13. A. Gopejenko

## Scientific visits abroad

Dr. hab. E. Kotomin, Max Planck Institute for Solid State Research, Stuttgart, Germany (9 months), Northwestern University, Evanston, USA (1 month), The Eurasian University, Astana, Kazakhstan (2 weeks)

Dr. hab. V. Kuzovkov, University of Freiburg, Germany (1 week)

Dr. O. Dumbrajs, Fukui University, Japan (3 months), Max Planck Institut für Plasmaphysik, Garching, Germany (3 months).

Dr. R. Eglitis, Rutgers University, USA (5 months)

Dr. V. Kashcheyevs, University of Cambridge, Cambridge, UK (1 week).

Dr. S. Piskunov, University of Duisburg-Essen (10 months), LNF Frascati, Italy (1 week)

Dr. A. Popov, Institute Laue-Langevin, Grenoble, France (3 months), National Laboratory of Frascati, Italy (10 days), Deutsches Elektronen-Synchrotron DESY Hamburg, Germany (10 days)

- Dr. D. Gryaznov, EC Institute of Transuranium Elements, Karlsruhe, Germany (10 months), Max Planck Institute for Solid State Physics, Stuttgart, Germany (1 month).
- Yu. Mastrikov, Max Planck Institute for Solid State Research, Stuttgart, Germany (11 months).
- Yu. Zhukovskii, Northwestern University, Evanston, USA (2 months), Max Planck Institute for Solid State Research, Stuttgart, Germany (3 weeks), Institute for Materials Research I, Karlsruhe (3 weeks), St. Petersburg State University, Russia (3 weeks), National Laboratory of Frascati, Italy (2 weeks).
- A. Gopejenko, Forschungszentrum Karlsruhe, Institut für Materialforschung I, Karlsruhe, Germany (5 months).

### Cooperation

|                  |   |
|------------------|---|
| <b>Finland</b>   | 1. Helsinki University of Technology (Dr. T. Kurki-Suonio)  |
| <b>France</b>    | 2. Laue-Langevin Institute, Grenoble (Dr. G.J. McIntyre, Dr. H.Schober)<br>3. ESRF, Grenoble (Dr. A.Rogalev)  |
| <b>Germany</b>   | 4. EC Institute of Transuranium Elements, Karlsruhe (Dr. P. van Uffelen).<br>5. Institut für Materialforschung I Forschungszentrum Karlsruhe (Dr. A. Möslang)<br>6. Universität Duisburg-Essen (Prof. Dr. E. Spohr)<br>7. Max Planck Institut für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier)<br>8. Max Planck Institut für Plasmaphysik, Garching (Prof. Dr. H. Zohm)<br>9. Physikalisch-Technische Bundesanstalt, Braunschweig (Dr. Bernd Kästner).<br>10. Deutsches Elektronen-Synchrotron DESY, Hamburg (Dr. A.Kotlov)<br>11. Institut für Hochleistungsimpuls & Mikrowellentechnik, Karlsruhe (Dr. B. Piosczyk)<br>Universität Ulm, Germany (Dr. T. Jacob) |
| <b>Greece</b>    | 13. School of Electrical and Computer Engineering, National Technical University of Athens, Zographou (Dr. Y. Kominis)  |
| <b>Israel</b>    | 14. Ben Gurion University of the Negev, Ber Sheeva (Profs. A. Aharony and D. Fuks)  |
| <b>Italy</b>     | 15. Laboratori Nazionali di Frascati (Dr. S. Bellucci, Dr.M.Cestelli-Guidi)   |
| <b>Japan</b>     | 16. FIR Center, University of Fukui (Prof. T. Idehara)  |
| <b>Lithuania</b> | 18. Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)   |
| <b>Romania</b>   | 19. University of Craiova (Dr. D. Constantinescu)   |
| <b>Russia</b>    | 20. St. Petersburg University (Prof. R.A. Evarestov)  |
| <b>Spain</b>     | 21. University of Barcelona (Prof. F. Illas)<br>22. Imperial College London (Prof. R.W. Grimes)   |
| <b>UK</b>        | 24. University College London (Profs. A.M. Stoneham and A. Shluger)<br>25. Cavendish Laboratory, University of Cambridge (M.R. Buitelaar)   |
| <b>Ukraine</b>   | 26. National University of Lviv (Prof. I. Bolesta and Prof. V. Savchyn)   |
| <b>USA</b>       | 27. Northwestern University, Evanston, Illinois (Prof. D.E. Ellis)<br>28. University of Maryland, College Park (Dr. G.S. Nusinovich, Dr M.Kukla)<br>Rutgers University (Prof. D. Vanderbilt)  |

## Main Results

### MODELING OF PHASE SEPARATION IN Au-Ni SURFACE ALLOY

G. Zvejnicks

E.E. Tornau (*Semiconductor Physics Institute, Vilnius, Lithuania*)

Detailed microscopic mathematical model of alloy phase separation can open new ways to optimize the Au/Ni surface catalyst. We proposed the kinetic Monte Carlo simulations of biatomic  $\text{Au}_{0.3}\text{Ni}_{0.7}$  surface alloy separation in Au/Ni(111) system by taking into account CO adsorption and nickel carbonyl formation reaction. We estimated Au-Au, Ni-Ni and Au-Ni pair interaction constants ( $v(\text{Au-Au})=-0.08$  eV,  $v(\text{Ni-Ni})=-0.39$  and  $v(\text{Au-Ni})=-0.25$ ) using *ab initio* calculations and find that they satisfy the inequality  $|v(\text{Au-Au})|+|v(\text{Ni-Ni})|<2|v(\text{Au-Ni})|$ . This condition ensures an increased Au concentration on step edge after alloy relaxation. In different limiting cases we have studied: (i) Step flow rate dependence on Au-CO interaction which is one of the main factors (along with CO pressure and reaction rate) governing the process of nickel carbonyl formation. (ii) Step flow rate delay with an increasing step edge Au concentration. (iii) Step flow rate increase with CO coverage,  $c_{\text{CO}}$ , which qualitatively agrees with the experiment only for  $c_{\text{CO}} \leq 0.45$  monolayer. (iv) We demonstrated both CO influence on reaction process and Au domain formation.

### ANDERSON LOCALIZATION: 2-D SYSTEM IN AN EXTERNAL MAGNETIC FIELD AND THE GENERALIZED DIFFUSION APPROACH

V. Kuzovkov

W. von Niessen (*TU Braunschweig, Germany*)

The analytical approach developed by us for the calculation of the phase diagram for the Anderson localization via disorder is generalized to the case of a strong magnetic field when  $q$  subbands ( $q=1,2,3$ ) arise. It is shown that in a line with the generally accepted point of view, each subband is characterized by a critical point with a divergent localization length  $\xi=1/\gamma(E,\sigma)$  which reveals anomaly in energy ( $E$ ) and disorder ( $\sigma$ ) parameters. These critical points belong to the phase coexistence area which cannot be interpreted by means of numerical investigations. The reason for this is a logical incompleteness of the algorithm used for analysis of a computer modelling for finite systems in the parameter range where the finite-size scaling is no longer valid.

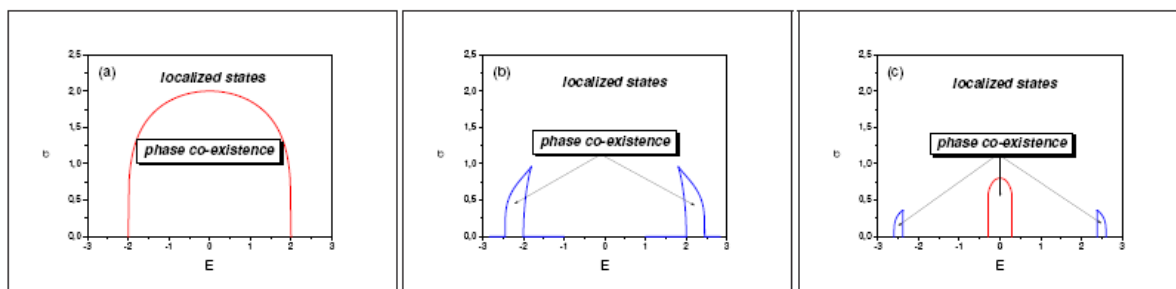


Figure 1 Phase diagram for  $q = 1$  (a),  $q = 2$  (b) and  $q = 3$  (c).

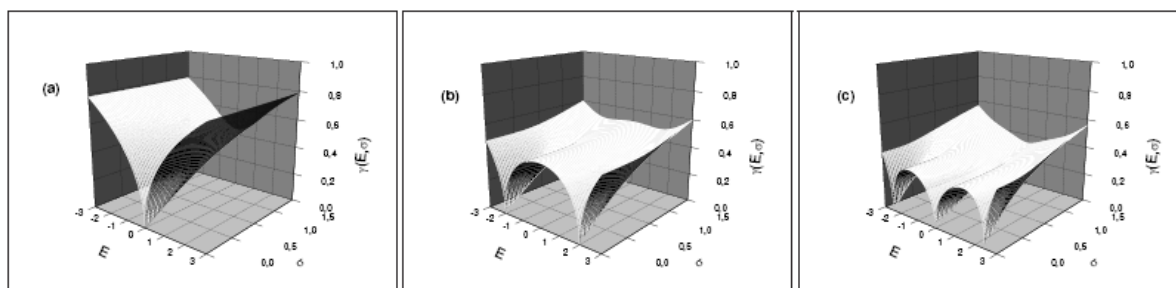


Figure 2 Surface plot  $\gamma(E, \sigma)$  for  $q = 1$  (a),  $q = 2$  (b) and  $q = 3$  (c).

## FIRST-PRINCIPLES CALCULATIONS OF PURE AND DEFECTIVE PEROVSKITE SURFACES

E.A. Kotomin, Yu. Zhukovskii, R.I. Eglitis, S. Piskunov, A. Gopeyenko,  
 E. Heifets (*Max Planck Institute, Germany*)  
 E. Spohr (*Universität Duisburg-Essen, Germany*)  
 T. Jacob (*Universität Ulm, Germany*)  
 D. E. Ellis (*Northwestern University, USA*)  
 D. Vanderbilt (*Rutgers University, USA*)

A wide class of ternary oxides –  $ABO_3$ -type perovskites – continues to attract a considerable attention as materials for catalytic and electrochemical applications, e.g. solid oxide fuel cells (SOFC), ceramic membranes for gas separation, actuators, sensors, *etc.* For example, some of these oxides are catalytically active in the oxidation of CO and reduction of NO in automobile exhaust reduction. Mixed oxides with the  $ABO_3$  perovskite structure are flexible systems as their properties can be adjusted or enhanced for specific applications by chemical doping at the A or B cation sites. Alternatively, these oxides can also contain *point defects* in the form of vacancies and trapped electrons/ holes depending on the A, B cation- and dopant nature. In all these applications surfaces play a key role.

In a close collaboration with prof. D.Vanderbilt (Rutgers University, USA), we performed *ab initio* calculations of a surface relaxation and rumpling for  $CaTiO_3$ ,  $SrTiO_3$  and  $PbZrO_3$  (001) as well as  $CaTiO_3$  and  $SrTiO_3$  (011) surfaces. The calculations are based on hybrid B3LYP exchange-correlation functionals. In the case of  $CaTiO_3$ , the surface rumpling is much larger for the CaO-terminated than for the  $TiO_2$ -terminated (001) surface, whereas different terminations of the  $CaTiO_3$  (011) surface lead to very different surface energies. Our calculations indicate a considerable increase in the Ti-O bond covalency near the TiO-terminated  $SrTiO_3$  (011) surface with respect to the bulk, which is much larger than that for the (001) surface.

In a close cooperation with Prof. D. Ellis (Northwestern University, USA), using the hybrid DFT-LCAO approach as implemented into the *CRYSTAL* code, we performed calculations of surface O vacancies with trapped electrons (known as the *F* centers) in three key perovskite crystals: SrTiO<sub>3</sub>, PbTiO<sub>3</sub> and PbZrO<sub>3</sub>. We have demonstrated that difference in a chemical composition of host materials leads to quite different defect properties: the *F* center is a shallow defect in titanates but a deep defect in zirconite. All three perovskites show a considerable trend in O vacancy segregation to the surfaces.

In a close cooperation with Prof. Spohr (Universität Duisburg-Essen, Germany), Dr. Heifets (Max Planck Institute, Germany), and Dr. Jacob (Universität Ulm, Germany), we have performed detailed calculations of the atomic, electronic structure and thermodynamic stability of La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> (LSM) solid solutions and its parent compound LaMnO<sub>3</sub> (LMO). Due to its high electrochemical performance, thermal and chemical stability, and

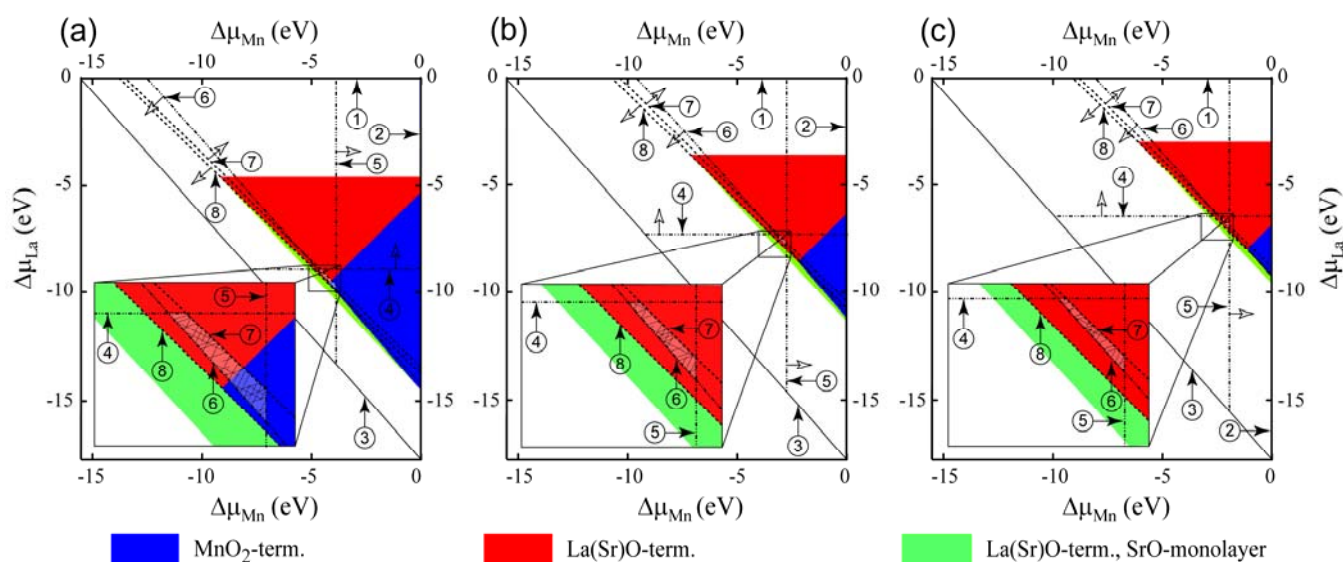


Fig. 1. Sections of thermodynamic stability diagram for LSM (001) surface structures for O<sub>2</sub> partial pressure ( $p = 0.2p_0$ ) and temperatures of (a) 300 K (room temperature), (b) 1100 K (SOFC operational temperature), and (c) 1500 K (sintering temperature). The region, where LSM ( $x = 1/8$ ) is stable, is the hatched area between LaMnO<sub>3</sub>, La<sub>2</sub>O<sub>3</sub>, Mn<sub>2</sub>O<sub>3</sub>, and SrO precipitation lines. The numbers from 1 to 8 in the circles indicate precipitation lines for (1) La, (2) Mn, (3) Sr, (4) La<sub>2</sub>O<sub>3</sub>, (5) Mn<sub>2</sub>O<sub>3</sub>, (6) SrO, (7) LaMnO<sub>3</sub>, and (8) SrMnO<sub>3</sub>. Hollow arrows indicate the sides from respective precipitation lines where the precipitation occurs. Insets show magnified areas with the region of LSM stability (a hatched quadrangle).

compatibility with yttria-stabilized zirconia (YSZ) electrolyte, LSM ( $x \approx 0.2$ ) has been actively used as a mixed ionic-electronic conducting electrode in high-temperature SOFC. Understanding the mechanism of reaction of oxygen reduction on the surface of LSM nanofilms deposited on oxide electrolytes demands thorough theoretical analysis at the atomistic level. In this study, first-principles calculations by means of a hybrid density-functional theory are used to describe La(Sr)O- and MnO<sub>2</sub>-terminated surfaces of both cubic LMO and LSM. Surfaces containing oxygen vacancies are also considered. Calculated thermodynamic stability diagrams (Fig. 1) predict that Sr-rich La(Sr)O-terminated LSM(001) become stable under conditions close to precipitation of SrMnO<sub>3</sub>. On the other hand, both La(Sr)O- and MnO<sub>2</sub>-terminated LSM(001) are stable at room temperature, while only La(Sr)O-terminated LSM(001) is predicted to be stable under SOFC operation conditions (temperature-gas pressure).

We predict a significant decrease in the O vacancy formation energy at higher temperatures which leads to a high vacancy concentration which permits efficient SOFC operation. The neutral oxygen vacancy attracts only  $\sim 0.6e$  and  $\sim 0.2e$  on La(Sr)O- and MnO<sub>2</sub>-terminated LSM (001), respectively. Thus, the vacancies are positively charged, they strongly polarize surrounding atoms and serve as potential adsorption

### POINT DEFECTS AND REACTIVITY OF ABO<sub>3</sub> PEROVSKITES

E.A. Kotomin, Yu. Zhukovskii, Yu. Mastrikov, S. Piskunov, A. Gopeyenko,

R.A. Evarestov, V. Alexandrov (*St. Petersburg University, Russia*)

D.E. Ellis (*Northwestern University, Evanston, USA*)

R. Merkle, V. Alexandrov, E. Heifets and J. Maier (*Max Planck Institute for Solid State Research, Stuttgart, Germany*)

We performed a series of first-principles (*ab initio*) calculations of defects in ABO<sub>3</sub>-type perovskites which is important for many high tech applications. In particular, in close collaboration with Max Planck Institute, Stuttgart we performed *ab initio* DFT plane-wave supercell calculations of the atomic and molecular oxygen adsorption and diffusion on the LaMnO<sub>3</sub> (001) surface which serves as a model material for a cathode of solid oxide fuel cells (SOFC). The calculations show that the dissociative adsorption of O<sub>2</sub> molecules from the gas phase is energetically favorable on surface Mn ions even on a defect-free surface.

The surface migration energy for adsorbed O ions is found to be quite high, 1.60 eV. We predict that the adsorbed O atoms could penetrate into electrode first plane when much more mobile surface oxygen vacancies (migration energy of 0.69 eV) approach the O ions strongly bound to the surface Mn ions. Formation of the O vacancy nearby O atom adsorbed atop surface Mn ion leads to an increase of the O-Mn binding energy by 0.74 eV whereas the drop of this adsorbed O atom into a vacancy possesses no energy barrier. As Fig.1 demonstrates the *ab initio* thermodynamics predicts that under typical SOFC operation temperatures ( $\sim 1200$  K) the MnO<sub>2</sub> (001) surface with adsorbed O atoms is the most stable in a very wide range of oxygen gas pressures (above  $10^{-2}$  atm). Second, in collaboration with Northwestern University, USA we performed *ab initio* calculations of Cu electrode growth on BaTiO<sub>3</sub> surfaces which important for micro-, nanoelectronic applications. In order to compare Cu adhesion upon two kinds of perfect cubic (001) oxide surfaces: (i) TiO<sub>2</sub>- and BaO-terminated substrates of partly covalent BaTiO<sub>3</sub> and (ii) highly ionic MgO substrate, we have performed DFT-LCAO calculations using a hybrid B3PW Hamiltonian. 2D symmetrical slabs used here contain seven BaTiO<sub>3</sub> and five MgO substrate layers covered on both sides by submonolayers of ordered Cu atoms. The Cu periodic coverage density atop the surface oxygen anions was varied from

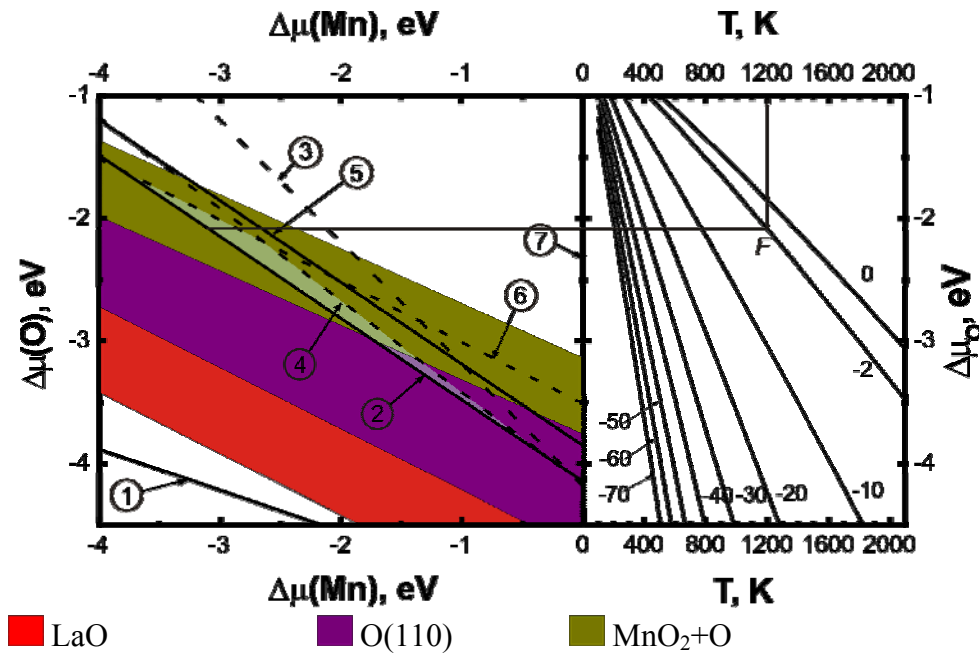


Fig.1. The stability diagram of different LaMnO<sub>3</sub> surfaces vs O<sub>2</sub> gas pressure (10<sup>-m</sup> atm.) and temperature. Numbers in circles indicate precipitation of metals and binary oxides.

1/8 to 1/2 monolayer. Copper bonding on the BaTiO<sub>3</sub>(001) surface has been found to be *noticeably stronger* than that on ionic MgO(001). Cu adatoms attract the electron density from BaO-terminated and donate it towards TiO<sub>2</sub>-terminated BaTiO<sub>3</sub>(001) substrates, respectively, by an amount that is about threefold larger than for a Cu/MgO(001) interface.

We performed also the hybrid LCAO calculations of Fe<sup>4+</sup> impurities substituting host Ti<sup>4+</sup> ions in the bulk and on the surface of SrTiO<sub>3</sub> varying iron concentration. The calculated local atomic deformation is in a good agreement with the EXAFS experimental data. We predict iron impurity segregation to the (001) surface which can contribute to the space charge effect and affect properties of internal interfaces and grain boundaries in ceramic samples.

We modelled also the external Li atom storage in nanocomposites known as the interfacial mechanism. This study is aimed to increase capacity and efficiency of Li batteries widely used in home electronics. To understand the mechanistic details of the experimentally observed lithium storage anomaly, we have performed comparative *ab initio* calculations on the atomic and electronic structure of the non-polar Cu/LiF(001) and model Li/LiF(001) interfaces. As we have shown the Cu/LiF(001) interface permits an insertion of only one monolayer of extra Li atoms, unlike Li bilayer in the case of Ti/Li<sub>2</sub>O(111). Diffusion of the excess Li along the interface is found to be accelerated owing to the splitting of the individual pathways for Li<sup>+</sup> and e<sup>-</sup>, which explains a high rate performance observed experimentally at low potential. We also compared theoretical estimate and experimental capacity results in the Cu/LiF nanocomposite.

The results of first-principles simulations on both orthorhombic and monoclinic phases of CaFeO<sub>3</sub> perovskite crystal were analysed. The obtained atomic structure is consistent with x-ray diffraction data. The transition from a metallic orthorhombic to a narrow-gap semiconducting monoclinic phase is ascribed to the larger distortion of the Fe-O-Fe bond angle in the latter case. Calculations of Raman and optic active phonon modes at the  $\Gamma$  point of the Brillouin zone are performed and discussed. The isotopic substitution technique is applied to analyze the vibration modes obtained. The found charge/spin disproportionation is analyzed and compared with available experimental estimates.



Lastly, point defects affect considerably properties of ABO<sub>3</sub>-type perovskite-based devices. One of the main defects is oxygen vacancy. In order to study its properties, we combined the hybrid DFT-LCAO approach with 135 atom supercell calculations of O vacancies with trapped electrons (known as the *F* centers) in three cubic perovskite crystals: SrTiO<sub>3</sub>, PbTiO<sub>3</sub> and PbZrO<sub>3</sub>. The local lattice relaxation, charge redistribution and defect energy levels in the optical gap were compared. We demonstrated how difference in chemical composition of host materials leads to quite different defect properties. The results obtained for three types of defective cubic ABO<sub>3</sub> perovskites show a strong defect property dependence on a chemical nature of A and B atoms: the same *F* centers could be deep defects in PbZrO<sub>3</sub> and shallow in SrTiO<sub>3</sub> and SrTiO<sub>3</sub>.

## FUNDAMENTAL AND APPLIED NANO-ELECTRONIC PUMPS

V. Kashcheyevs

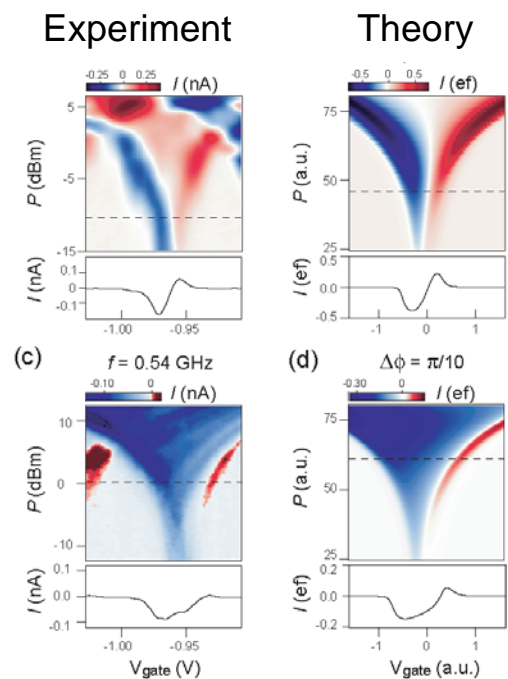
M.R. Buitelaar (*Cavendish Laboratory, University of Cambridge, UK*)

B. Kästner (*Physikalisch-Technische Bundesanstalt, Braunschweig, Germany*)

Quantum electron pumps, based of periodic modulation of quantum dot parameters, is a rapidly developing class of nanoelectronic devices. Fundamental applications involve probing of electron excitation spectrum and quantum information processing while the main applied interest is the development of a quantum current standard.

In *collaboration with the experimental group at University of Cambridge (Dr. Markk Buitelaar ,Cambridge, UK)*, we have identified signatures of a artificial molecule states in carbon-nanotube based adiabatic pump [3], see the figure. This work has been recognized as one of the **top 10 science achievements in Latvia in 2008** by the Latvian Academy of Sciences (the annual ‘Top 10’ covers all branches of science, from medicine to lettonica to physics). In *collaboration with the experimental group at Physikalisch-Technische Bundesanstalt (Dr. Bernd Kästner, Braunschweig, Germany)* we have continued work on a novel non-

adiabtic architecture for a quantized source of current (quantized pumping) [1,2]. Application of magnetic field has allowed to achieve the highest accuracy of current quantization to date. We continue theoretical work towards optimizing this architecture towards metrological accuracy (100 parts per billion).



## HYSTERESIS IN MODE COMPETITION IN HIGH POWER 170 GHz GYROTRON FOR ITER

O. Dumbrajs

T. Idehara (*University of Fukui, Japan*)

Gyrotrons are microwave sources whose operation is based on the stimulated cyclotron radiation of electrons oscillating in a static magnetic field. Gyrotron devices are now able to generate several orders of magnitude as much power at millimeter wavelength as classical microwave tubes, and can operate at frequencies higher than are conveniently available from other types of tubes. Gyrotron oscillators can have a wide application,



including technological processes, atmospheric sensing, ozone conservation, artificial ionospheric mirror, extra-high resolution electron spin resonance spectroscopy, nuclear magnetic resonance spectroscopy, new medical technology spectroscopy, etc. However, the main application of powerful gyrotrons is electron cyclotron resonance plasma heating in tokamaks and stellarators and the noninductive current drive in tokamaks.

The study of one very interesting phenomenon—hysteresis—is relatively limited, although perfect understanding of hysteresis is important in connection with mode competition, frequency tuning, voltage overshooting, amplitude modulation of the signal, etc. In gyrotrons hysteresis is the phenomenon that causes the amplitude of oscillations to lag behind the magnetic field and the voltage, so that operation regions of modes for rising and falling magnetic field and voltage are not the same.

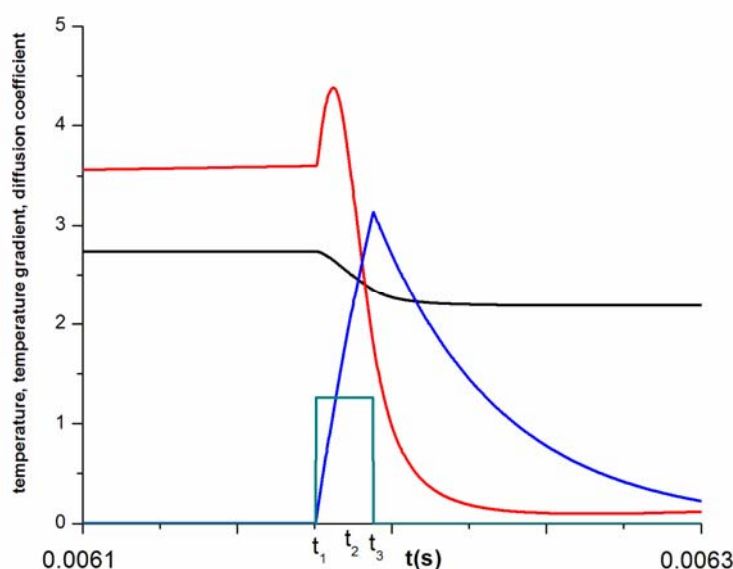
In the present work, we generalize our single mode hysteresis calculations to multimode case with particular emphasis on mode competition in 170 GHz gyrotrons for ITER and calculate mode map in the plane “frequency mismatch – dimensionless current” for the operating mode. The theory is illustrated by a number of specific examples.

## HYSTERESIS IN SAWTOOTH CRASH IN ASDEX UPGRADE TOKAMAK

O. Dumbrajs

V. Igochine, H. Zohm and ASDEX Upgrade Team (*MPI für Plasmaphysik, Euratom-Association, D-85748 Garching, Germany*)

A hysteresis model is used to describe experimental data on sawtooth crash in ASDEX Upgrade tokamak. The model is based on hysteresis which arises due to the fact that the value of the current density gradient (approximated, for the H-mode discharges studied here, by the temperature gradient) at the  $q = 1$  surface required to turn on the instability is greater than the gradient required to maintain the instability once it is turned on. The value of the hysteresis parameter can be chosen such that the model reproduces correctly the two time scales of the sawtooth crash in ASDEX Upgrade tokamak: the slow rise time ( $\sim 7$  ms) and the rapid crash time ( $\sim 50$   $\mu$ s).



Hysteresis in sawtooth crash. Temperature gradient (red curve) rises until the instability threshold at  $3.6$  keV/m. At this moment  $t = t_1$  the instability is turned on by switching the function  $Q$  (green curve, arbitrary units) to  $\chi_{\max}$ . The central temperature (black

curve) begins to decrease and diffusion coefficient (blue curve, arbitrary units) begins to increase. During further evolution due to hysteresis the function  $Q$  is switched back to  $\chi_{\min}$  not at  $t = t_2$  when temperature gradient passes again the instability threshold, but at  $t = t_3$  when temperature gradient becomes equal to  $\beta k = 1.8 \text{ keV/m}$ .

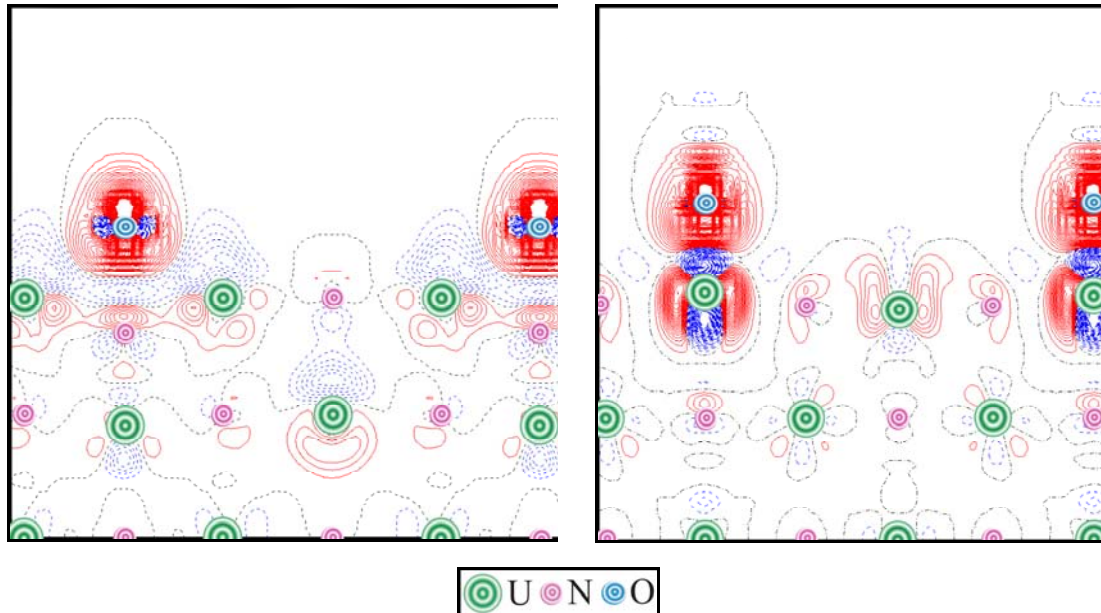
## AB INITIO MODELLING OF ADVANCED NUCLEAR FUEL OXIDATION

E.A. Kotomin, Yu. Zhukovskii, Yu. Mastrikov, D. Gryaznov, D. Bocharov,  
 R.A. Evarestov, A.V. Bandura, M.V. Losev (*Department of Quantum Chemistry, St. Petersburg State University, St. Petersburg, Russia*)  
 P. Van Uffelen (*Institute of Transuranium Elements, Karlsruhe, Germany*),

In close collaboration with the *Institute for Transuranium Elements, Karlsruhe*, we have continued first-principles calculations of UN fuels. Uranium mononitride attracts a considerable attention as promising nuclear fuel materials for future Generation IV reactors. In order to predict nuclear fuel performance under different operating conditions and then during a prolonged time in repository for a spent fuel, it is necessary to understand and predict material physico-chemical properties.

Theoretical studies of uranium compounds are especially difficult due to a relativistic character of electron motion in the U atom core and strong electron-electron correlation. Moreover, UN is characterized by a mixed metal-covalent chemical bonding.

***UN samples typically contain considerable amount of O impurities, which greatly affect fuel properties. Therefore, it is necessary to understand mechanism of oxygen adsorption as well as further oxidation of uranium nitride.***



***Fig. 1. The difference electron density maps  $\Delta\rho(r)$  (the total density of the interface minus the densities of substrate and adsorbate with optimized interfacial geometry) for the O adatoms atop the surface: (left) N anions and (right) U cations on the UN(001) surface obtained using results of calculations. Solid (red) and dashed (blue) isolines correspond to positive and negative electron density, respectively. Isodensity increment is  $0.003 e \text{ \AA}^{-3}$ .***

The results of PW DFT calculations of the lattice constant, bulk modulus, cohesive energy, charge distribution, band structure and density of states (DOS) for UN pure bulk and surface are analysed. The DFT plane wave (PW) calculations on a pure

UN bulk and surface as well as oxygen atomic absorption on defect-free UN surface were compared with the corresponding LCAO DFT calculations performed by Prof. R.A. Evarestov group (*Faculty of Chemistry, St. Petersburg State University*). The results acquired for oxygen interaction with UN surfaces demonstrate a strong chemisorption typical for metallic surfaces. An analysis of the difference electron charge redistributions for both configurations of  $O_{\text{ads}}$  (Fig. above) confirms that the O adatom forms a strong chemical bonding with the surface U cation which could be considered as one-site complex. In the case of O adatom atop the surface N anion this is rather multi-center adsorption complex involving four adjacent surface U ions. A comparison of the DFT GGA with LCAO calculations shows their excellent agreement.

DFT PW calculations show also that O impurities are able to penetrate easily into the UN in bulk and oxidize the fuel which agrees well the results of experimental studies. The oxygen incorporation into (pre-existing) N vacancy is energetically more favorable than that into the tetrahedral interstitial position. However, it is energetically favorable even to create N vacancy and place O atom therein.

Based on the GGA calculations, we demonstrated that  $O_2$  molecules oriented parallel to the UN substrate can dissociate either (*i*) spontaneously, when the molecule center lies above the surface hollow site or atop N ion, or (*ii*) with the activation barrier, when a molecule sits atop the surface U ion. This explains fast UN oxidation in air. A study of He impurities are in progress.

## **SIMULATION OF YTTRIUM AND OXYGEN SOLUTE ATOMS IN FCC FE LATTICE IN SUPPORT OF ODS STEEL DEVELOPMENT**

A.Gopejenko, Yu.F. Zhukovskii, E.A.Kotomin,  
P.V.Vladimirov and A.Möslang (*Forschungszentrum Karlsruhe, Institut für  
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Reduced activation steels strengthened by yttria precipitates are considered as promising structural materials for future fusion- and advanced fission-reactors. In particular, application of oxide dispersion strengthened (ODS) steels for fusion reactor blanket structure allows increasing its operation temperature by  $\sim 100^\circ\text{C}$ . Both size and spatial distributions of oxide precipitates significantly affect mechanical properties and radiation resistance of ODS steels. However, the mechanism of ODS nanoparticle formation is still not well understood. Some recent experiments indicate that at least part of yttrium oxide particles might be dissolved in the steel matrix during mechanical alloying. If so, yttrium dissolved above its equilibrium solubility limit will precipitate during hot isostatic pressing of mechanically alloyed powder. Slow diffusion of large substitutional yttrium atoms is probably a limiting factor for yttrium oxide particle growth. Diffusion of interstitial oxygen is much faster and, therefore, can not delay the growth of precipitate. In this paper we consider an Y-vacancy pair as a simplest diffusing yttrium-containing complex.

In collaboration with *Institute for Materials Research I, Research Center Karlsruhe*, we have performed a series of large-scale first principles calculations on perfect  $\gamma$ -Fe lattice as well as that containing a single Fe atom vacancy, O and Y impurity atoms. In our model iron matrix is represented by a face-centered cubic  $\gamma$ -Fe lattice, which is stable at typical hot isostatic pressing temperatures. Our calculations performed for the  $4\times 4\times 4$   $\gamma$ -Fe supercell have shown that oxygen atoms reside on either *O* (six nearest Fe neighbors) or *T* (four nearest Fe neighbors) interstitial positions (the latter has been found to be  $\sim 0.1$ - $0.2$  eV less favorable than the former) which quantitatively confirm results of theoretical simulations on oxygen atom absorbed inside the fcc Al lattice. The excessive electronic charge accepted by oxygen impurity in O center of  $\gamma$ -Fe lattice achieves  $\sim 1.4$  e (cf. 1.8 e for the same position of O atom in fcc Al lattice). The oxygen

insertion results in a considerable expansion of the two first coordination shells around an impurity atom (~9 and 1.75%, respectively, in octahedral interstitial). A barrier of O migration between the nearest O and T centers (1.62 eV) has been found in a good qualitative agreement with the corresponding experimental values (1.72-1.75 eV, according to different studies). Our calculations have shown that there is a considerable binding between yttrium atom and vacancy at some distances (Figures 1a and 1b). This allows us to determine the pair-wise energies necessary for further kinetic Monte Carlo simulations, aimed at understanding the yttrium oxide precipitation process.

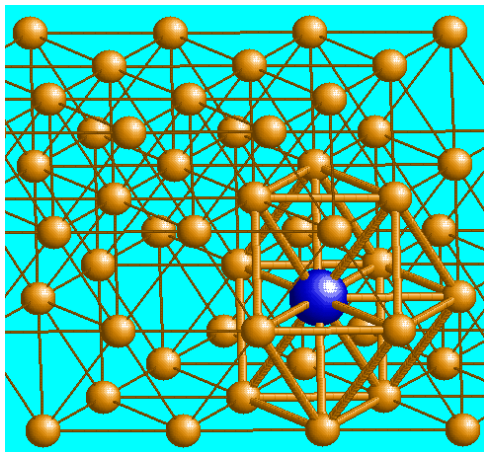


Figure 1a. Configuration of the Y and Fe-vacancy pair at 1NN position before relaxation

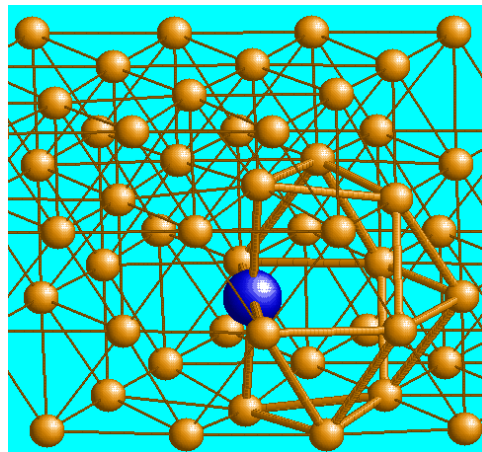


Figure 1b. Configuration of the Y and Fe-vacancy pair at 1NN position after relaxation

### MICROSTRUCTURE OF $\text{Ag}_2\text{BI}_4$ (B =Hg, Cd) SUPERIONICS STUDIED BY SEM, IMPEDANCE SPECTROSCOPY AND FRACTAL DIMENSION ANALYSIS

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Two silver ion conducting solid electrolytes,  $\text{Ag}_2\text{HgI}_4$  and  $\text{Ag}_2\text{CdI}_4$ , representing a wide class of AgI-based halogenide superionics have been the subjects of study by means of electrical impedance spectroscopy, SEM, porosity measurements and fractal dimension analysis. Even though both materials have been obtained by the same method under strictly identical conditions they were found to exhibit certain differences at the microstructural level. Thus, by the direct measurements of porosity and density it was found that the grain boundaries are better developed in silver mercuric iodide. On the assumption that pore geometry in the materials under study displays fractal character it was shown that the fractal dimension of the pore contours is larger in the case of  $\text{Ag}_2\text{HgI}_4$ . These results are in agreement with electrical studies which indicated that the



grain boundary capacitance in  $\text{Ag}_2\text{CdI}_4$  is two orders of magnitude smaller than that of the silver mercuric iodide.

## **AB INITIO SIMULATIONS ON THE ATOMIC AND ELECTRONIC STRUCTURE OF REGULAR AND DEFECTIVE SINGLE-WALLED BN NANOTUBES AND NANOARCHES**

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To simulate the perfect single-walled (SW) boron nitride (BN) nanotubes (NTs) and nanoarches (NAs) of armchair- and zigzag-type chiralities as well as uniform diameter we have constructed their 1D-periodic models, in the framework of collaboration with the *LNF INFN, Frascati, and Politecnico di Torino, Italy*. In the NAs of both chiralities, the half-NTs have been extended by two fragments of parallel nanoribbons joint to their edges. The nanotubes and nanoarches have been calculated using formalism of the localized Gaussian-type atomic functions as implemented in the *CRYSTAL-06* code. For *ab initio* calculations, we have applied the DFT Hamiltonians containing either PWGGA or hybrid (DFT+HF) B3PW exchange-correlation functionals. We have compared the calculated both structural and electronic properties of BN NTs and NAs with those for *h*-BN and *c*-BN bulk. After calculation of Hessian matrix for the optimized structures of BN bulk (both phases) and nanotubes (both chiralities) using the *CRYSTAL* code we have estimated their normal phonon modes within the harmonic approximation. Applying both atomistic and continuum models we have calculated the elastic energies and moduli for SW BN nanoarches. Their careful study is necessary not only for reliable comparison with the corresponding experimental data but also for proper description and even prediction for some of them (firstly, the phonon and elastic structure of BN nanotubes and nanoarches). Recent experimental IR measurements on *h*-BN and BN NT samples qualitatively confirmed the spectra predicted in this study. The hybrid B3PW method is found to be more reliable for the simulation of the whole spectrum of properties for BN bulk and nanostructures.

Using the hybrid B3PW method for *ab initio* calculations in collaboration with the *LNF INFN, Frascati*, we have also simulated the relaxed structure, the electron charge re-distribution and the energetics of neutral nitrogen vacancy (*F* center) as well as  $\text{C}_\text{N}$  and  $\text{O}_\text{N}$  substitutes in BN nanotubes. All three types of point defects cause an appearance of the energy levels inside the BN NT band gap (Fig. 1) accompanied by relaxation of the nearest atomic spheres closest to the point defect and electronic charge redistribution around it. Energetically, formation of carbon and oxygen substitutes in BN NTs is more preferable than that for N vacancy.  $\text{C}_\text{N}$  point defects serve as electron acceptors making BN nanotube a *p*-type semiconductor. Oxygen substitutes are typical electron donors in BN NT and in the case of its *zz*-chirality they show a metallic behavior. We also can conclude that different nature of chemical bonding in nanotubes of III group metal nitrides can result in a noticeable difference between their properties, especially in presence of defects.

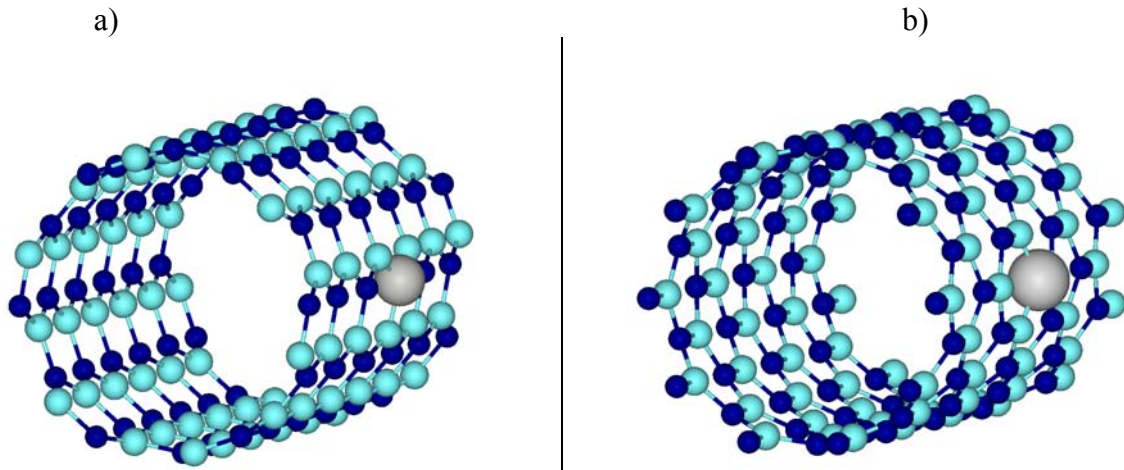


Figure 1. Aside views of periodic fragments of  $\sim 8.5$  Å thick 1D BN NTs containing single defects ( $F$  center,  $C_N$  and  $O_N$ ) distributed along axes of nanotube upon: a)  $ac$ -NT (6,6) with supercell periodicity 16.2 Å and b)  $zz$ -NT (10,0) with supercell periodicity 17.3 Å. Large light-gray balls show single defects ( $F$  centers,  $C_N$ ,  $O_N$ ) whereas light turquoise balls correspond to B atoms and N atoms are shown by dark blue.

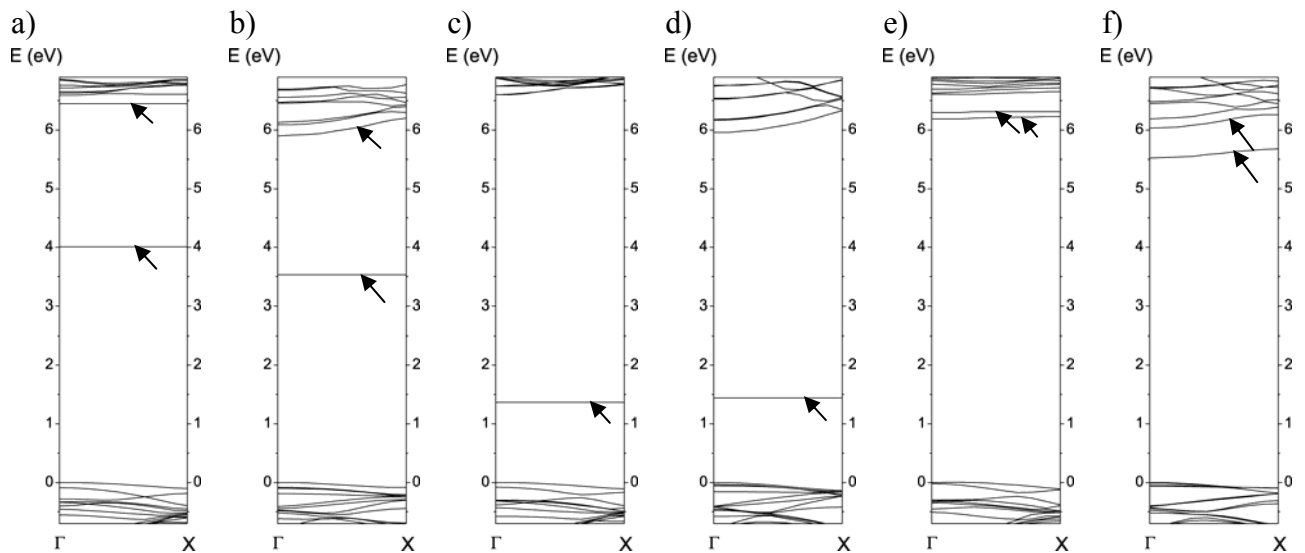


Figure 2. Band structures of BN NTs containing a single defect *per* supercell:  $F$  center upon  $ac$ -NT (a) and  $zz$ -NT (b);  $C_N$  upon  $ac$ -NT (c) and  $zz$ -NT (d);  $O_N$  upon  $ac$ -NT (e) and  $zz$ -NT (f). Arrows show the defect bands whereas zero level in all the energy scales is chosen at the top VB.

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2. V. Kashcheyevs, C. Karrasch, T. Hecht, and V. Meden, "From single particle to correlation-dominated criticality in a level-crossing transition". Abstracts: Po. 22.

#### ***III. 24<sup>th</sup> ISSP Conference (Riga, Latvia, February, 2008).***

3. A. Gopejenko, Yu.F Zhukovskii, P.V. Vladimirov, and E.A. Kotomin, "Ab initio calculations of O and Y impurities in Fe fcc lattice". Abstracts: p. 4.

4. D. Bocharov, Yu.F. Zhukovskii, D. Gryaznov, R.A. Evarestov, E.A. Kotomin, "Structure and properties of UN nuclear fuels: quantum chemistry approach". Abstracts: p. 6.

5. O. Dumbrajs, "Gyrotrons for ITER". Abstracts: p. 27.

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6. S. Piskunov, E. Spohr, and T. Jacob, "Electronic structure and thermodynamic stability of cubic La<sub>1-x</sub>Sr<sub>x</sub>MnO<sub>3</sub> (001) surfaces: First principles calculations by means of hybrid density-functional theory". Abstracts: p. 592-593.

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8. O. Dumbrajs, "Stochastic processes in gyrotrons".

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11. Yu.F. Zhukovskii, S. Piskunov, B. Berzina, L. Trinkler, and S. Bellucci, "Atomic

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12. A.I. Popov, G.J. McIntyre, C. Wilkinson, "Photostimulable storage phosphors and image-plate development for neutron imaging". Abstracts: p. 32.

13. D. Bocharov, Yu. Zhukovskii, R.A. Evarestov, E.A. Kotomin, and A. Bandura, "Atomic and molecular oxygen adsorption on the UN (001) surface". Abstracts: p. 87.

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23. D. Bocharov, Yu.F. Zhukovskii, and E.A. Kotomin, "Spontaneous dissociation of  $\text{O}_2$  molecules at oxygen adsorption on the UN(001) surface". Abstracts: p. 14.

24. A. Gopeyenko, Yu.F. Zhukovskii, P.V. Vladimirov, and E.A. Kotomin, "*Ab initio* Calculations of oxygen and yttrium impurities in *fcc* Fe". Abstracts: p. 23.

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