

**Janis Timoshenko**  
**LIST OF PUBLICATIONS**

**RESEARCHER-ID: F-1027-2010**  
**ORCID 0000-0003-2963-3912**

**2021**

INFLUENCE OF THE COBALT CONTENT IN COBALT IRON OXIDES ON THE ELECTROCATALYTIC OER ACTIVITY

S. Saddeler, G. Bendt, S. Salamon, F. Haase, J. Landers, **J. Timoshenko**, C. Rettenmaier, H. Jeon, A. Bergmann, H. Wende, B. Roldan Cuenya and S. Schulz.

J. Mat. Chem. A, *in press*.

AMORPHOUS P-TYPE CONDUCTING Zn<sub>1-x</sub>Ir OXIDE (x>0.13) THIN FILMS DEPOSITED BY REACTIVE MAGNETRON COSPUTTERING

M. Zubkins, **J. Timoshenko**, J. Gabrusenoks, K. Pudzs, A. Azens, Q. Wang, J. Purans

Phys. Status Solidi B, *in press*.

THEORETICAL AND EXPERIMENTAL STUDIES OF CHARGE ORDERING IN CaFeO<sub>3</sub> AND SrFeO<sub>3</sub> CRYSTALS

E. A. Kotomin, A. Kuzmin, J. Purans, **J. Timoshenko**, S. Piskunov,

Phys. Status Solidi B, *in press*.

SELECTIVITY CONTROL OF CU NANOCRYSTALS IN A GAS-FED FLOW CELL THROUGH CO<sub>2</sub> PULSED ELECTROREDUCTION

H. Jeon, **J. Timoshenko**, C. Rettenmaier, A. Herzog, A. Yoon, S.W. Chee, S. Oener, U. Hejral, F. Haase and B. Roldan Cuenya.

J. Am. Chem. Soc. 143 7578 (2021)

ROLE OF THE OXIDE SUPPORT ON THE STRUCTURAL AND CHEMICAL EVOLUTION OF FE CATALYSTS DURING THE HYDROGENATION OF CO<sub>2</sub>

M. Lopez-Luna, J. Timoshenko, D. Kordus, C. Rettenmaier, S.W. Chee, A.S. Hoffman, S.R. Bare, S.K. Shaikhutdinov and B. Roldan Cuenya

ACS Catal. 11 6175 (2021).

IN SITU/OPERANDO ELECTROCATALYST CHARACTERIZATION BY X-RAY ABSORPTION SPECTROSCOPY

**J. Timoshenko**, B. Roldan Cuenya

Chem. Rev. 121 882 (2021)

Pt-Sn-Co NANOCUBES AS HIGHLY ACTIVE CATALYSTS FOR ETHANOL ELECTRO-OXIDATION

R. Rizo, A. Bergmann, **J. Timoshenko**, F. Scholten, C. Rettenmaier, H. Jeon, Y.-T. Chen, A. Yoon, A. Bagger, J. Rossmeisl and B. Roldan Cuenya

J. Catal. 393 247 (2021)

OPERANDO HIGH-PRESSURE INVESTIGATION OF SIZE-CONTROLLED CuZn CATALYSTS FOR THE METHANOL SYNTHESIS REACTION

N.J. Divins, D. Kordus, **J. Timoshenko**, I. Sinev, I. Zegkinoglou, A. Bergmann, S.W. Chee, S. Widrinna, O. Karshloğlu, H. Mistry, M. Lopez Luna, J.Q. Zhong, A.S. Hoffmann, A. Boubnov, J.A. Boscoboinik, M. Heggen, R.E. Dunin-Borkowski, S.R. Bare and B. Roldan Cuenya  
Nature Commun. 12 1435 (2021)

OPERANDO INVESTIGATION OF Ag-DECORATED Cu<sub>2</sub>O NANOCUBE CATALYSTS WITH ENHANCED CO<sub>2</sub> ELECTROREDUCTION TOWARD LIQUID PRODUCTS.  
A. Herzog, A. Bergmann, H. Jeon, **J. Timoshenko**, S. Kühn, C. Rettenmaier, M. Lopez-Luna, F. Haase and B. Roldan Cuenya  
Angew. Chem. 60 7426 (2021)

## 2020

LINKING THE EVOLUTION OF CATALYTIC PROPERTIES AND STRUCTURAL CHANGES IN COPPER-ZINC NANOCATALYSTS USING OPERANDO EXAFS AND NEURAL-NETWORKS  
**J. Timoshenko**, H. S. Jeon, I. Sinev, F. Haase, A. Herzog, B. Roldan Cuenya  
Chem. Sci. 11 3727 (2020)

ELECTROCATALYTIC CO<sub>2</sub> REDUCTION ON CuO<sub>x</sub> NANOCUBES: TRACKING THE EVOLUTION OF CHEMICAL STATE, GEOMETRIC STRUCTURE, AND CATALYTIC SELECTIVITY USING OPERANDO SPECTROSCOPY  
T. Moller, F. Scholten, T.N. Thanh, I. Sinev, **J. Timoshenko**, X.L. Wang, Z. Jovanov, M. Gliech, B. Roldan Cuenya, A.S. Varela, P. Strasser  
Angew. Chem. 59 17974 (2020)

ENHANCED FORMIC ACID OXIDATION OVER SnO<sub>2</sub>-DECORATED Pd NANOCUBES  
C. Rettenmaier, R. Aran Ais, **J. Timoshenko**, R. Rizo, H. Jeon, S. Kühn, S.W. Chee, A. Bergmann and B. Roldan Cuenya  
ACS Catal. 10 14540 (2020)

OPERANDO NRIXS AND XAFS INVESTIGATION OF SEGREGATION PHENOMENA IN FE-CU AND FE-AG NANOPARTICLE CATALYSTS DURING CO<sub>2</sub> ELECTROREDUCTION  
S. Kunze, P. Grosse, M.B. Lopez, I. Sinev, I. Zegkinoglou, H. Mistry, **J. Timoshenko**, M.Y. Hu, J. Zhao, E.E. Alp, S.W. Chee and B. Roldan Cuenya  
Angew. Chem. 50 22667 (2020)

KEY ROLE OF CHEMISTRY VERSUS BIAS IN ELECTROCATALYTIC OXYGEN EVOLUTION  
H.N. Nong, L. Falling, A. Bergmann, M. Klingenhof, H.P. Tran, C. Spöri, R. Mom, **J. Timoshenko**, G. Zichittella, A. Knop-Gericke, S. Piccinin, J. Pérez-Ramírez, B. Roldan Cuenya, R. Schlögl, P. Strasser, D. Teschner and T. Jones  
Nature 587 408 (2020)

NEURAL NETWORK ASSISTED ANALYSIS OF BIMETALLIC NANOCATALYSTS USING X-RAY ABSORPTION NEAR EDGE STRUCTURE SPECTROSCOPY

N. Marcella, Y. Liu, **J. Timoshenko**, E.J. Guan, M. Luneau, T. Shirman, A.M. Plonka, J.E.S. van der Hoeven, J. Aizenberg, C.M. Friend, A.I. Frenkel  
Phys. Chem. Chem. Phys. 22 18902 (2020)

INSIGHT INTO RESTRUCTURING OF Pd-Au NANOPARTICLES USING EXAFS.

A. Boubnov, **J. Timoshenko**, C. J. Wrasman, A. S. Hoffman, M. Cargnello, A. I. Frenkel, S. R. Bare  
Rad. Phys. Chem. 175 108304 (2020)

SILVER CLUSTERS SHAPE DETERMINATION FROM IN-SITU XANES DATA

**J. Timoshenko**, S. Roese, H. Hovel, A. I. Frenkel  
Rad. Phys. Chem. 175 108049 (2020)

TREATMENT OF DISORDER EFFECTS IN X-RAY ABSORPTION SPECTRA BEYOND THE CONVENTIONAL APPROACH

A. Kuzmin, **J. Timoshenko**, A. Kalinko, I. Jonane, A. Anspoks  
Rad. Phys. Chem. 175 108112 (2020)

LOCAL STRUCTURE OF A-ATOM IN ABO<sub>3</sub> PEROVSKITES STUDIES BY RMC-EXAFS

A. Anspoks, C. Marini, T. Miyanaga, B. Joseph, A. Kuzmin, J. Purans, **J. Timoshenko**, A. Bussmann-Holder  
Rad. Phys. Chem. 175 108072 (2020)

INTERPRETATION OF THE Cu K-EDGE EXAFS SPECTRA OF Cu<sub>3</sub>N USING AB INITIO MOLECULAR DYNAMICS

D. Bocharov, A. Anspoks, **J. Timoshenko**, A. Kalinko, M. Krack, A. Kuzmin  
Rad. Phys. Chem. 175 108100 (2020)

MACHINE-LEARNING ASSISTED DETERMINATION OF COORDINATION NUMBERS OF METALLIC NANOPARTICLES – A BENCHMARK,

Y. Lin, M. Topsakal, **J. Timoshenko**, D. Lu, S. Yoo, A. I. Frenkel  
Chapter in *Handbook on Big Data and Machine Learning in the Physical Sciences*, World Scientific Series on Emerging Technologies, v.2, Chapter 7, pp. 127-140 (2020)

## 2019

OPERANDO INSIGHT INTO THE CORRELATION BETWEEN THE STRUCTURE AND COMPOSITION OF CuZn NANOPARTICLES AND THEIR SELECTIVITY FOR THE ELECTROCHEMICAL CO<sub>2</sub> REDUCTION

H. S. Jeon, **J. Timoshenko**, F. Scholten, I. Sinev, A. Herzog, F. Haase, B. Roldan Cuenya  
J. Am. Chem. Soc. 141, 19879 (2019)

SELECTIVE CO<sub>2</sub> ELECTROREDUCTION TO ETHYLENE AND MULTICARBON ALCOHOLS VIA ELECTROLYTE-DRIVEN NANOSTRUCTURING

D. Gao, I. Sinev, F. Scholten, R. M. Arán-Ais, N. J. Divins, K. Kvashnina, **J. Timoshenko**, B. Roldan Cuenya

Angew. Chem. Int. Ed. 58, 17047 (2019).

IS THERE A NEGATIVE THERMAL EXPANSION IN SUPPORTED METAL NANOPARTICLES?: AN IN SITU X-RAY ABSORPTION STUDY COUPLED WITH NEURAL NETWORK ANALYSIS

**J. Timoshenko**, M. Ahmadi, B. Roldan Cuenya

J. Phys. Chem. C 123, 20594 (2019).

TUNING THE STRUCTURE OF Pt NANOPARTICLES THROUGH SUPPORT INTERACTIONS: AN IN SITU POLARIZED X-RAY ABSORPTION STUDY COUPLED WITH ATOMISTIC SIMULATIONS

M. Ahmadi, **J. Timoshenko**, F. Behafarid, B. Roldan Cuenya

J. Phys. Chem. C 123, 10666 (2019)

“INVERTING” X-RAY ABSORPTION SPECTRA OF CATALYSTS BY MACHINE LEARNING IN SEARCH FOR ACTIVITY DESCRIPTORS

**J. Timoshenko**, A. I. Frenkel

ACS Catal. (Perspective) 9, 10192 (2019)

MAPPING XANES SPECTRA ON STRUCTURAL DESCRIPTORS OF COPPER OXIDE CLUSTERS USING SUPERVISED MACHINE LEARNING

Y. Liu, N. Marcella, **J. Timoshenko**, A. Halder, B. Yang, L. Kolipaka, M. J. Pellin, S. Seifert, S. Vajda, P. Liu, A. I. Frenkel

J. Chem. Phys. 151, 164201 (2019)

**(JCP Editors' Pick)**

LOCAL STRUCTURE AND ELECTRONIC STATE OF ATOMICALLY DISPERSED PT ON NANOSIZED CeO<sub>2</sub> SUPPORT

M. Kottwitz, Y. Li, R. M. Palomino, Z. Liu, Q. Wu, G. Wang, J. Huang, **J. Timoshenko**, S. D. Senanayake, M. Balasubramanian, D. Lu, R. G. Nuzzo, A. I. Frenkel

ACS Catalysis 9, 8738 (2019)

DILUTE Pd/Au ALLOY NANOPARTICLES EMBEDDED IN COLLOID TEMPLATED POROUS SiO<sub>2</sub>: STABLE Au-BASED OXIDATION CATALYSTS

M. Luneau, T. Shirman, A. Filie, **J. Timoshenko**, W. Chen, A. Trimpalis, M. Flytzani-Stephanopoulos, E. Kaxiras, A. I. Frenkel, J. Aizenberg, C. M. Friend, R. M. Madix

Chem. Mater. 31, 5759 (2019)

MODELING STRAIN DISTRIBUTION AT THE ATOMIC LEVEL IN DOPED CERIA FILMS WITH EXTENDED X-RAY ABSORPTION FINE STRUCTURE SPECTROSCOPY

O. Kraynis, **J. Timoshenko**, J. Huang, H. Singh, E. Wachtel, A. I. Frenkel, I. Lubomirsky

Inorg. Chem. 58 7527 (2019)

SOLVING THE STRUCTURE AND DYNAMICS OF METAL NANOPARTICLES BY COMBINING X-RAY ABSORPTION FINE STRUCTURE SPECTROSCOPY AND ATOMISTIC STRUCTURE SIMULATIONS

**J. Timoshenko**, Z. Duan, G. Henkelman, R. M. Crooks, A. I. Frenkel

Annu. Rev. Anal. Chem 12, 501 (2019)

DESIGNING NANOPATELET ALLOY/NAFION MEMBRANES FOR OPTIMIZATION OF PEMFCS PERFORMANCE: OPERATION, DURABILITY, AND CO RESISTANCE

L. Wang, Y. Zhou, **J. Timoshenko**, S. Liu, Q. Qiao, K. Kisslinger, M. Cuiffo, Y. Chuang, X. Zuo, Y. Xue, C. Pan, H. Li, C.-Y. Nam, S. Bliznakov, P. Liu, A. I. Frenkel, Y. Zhu, M. Rafailovich  
ACS Catalysis 9, 1446 (2019)

PROBING ATOMIC DISTRIBUTIONS IN MONO- AND BIMETALLIC NANOPARTICLES BY SUPERVISED MACHINE LEARNING

**J. Timoshenko**, C. J. Wrasman, M. Luneau, T. Shirman, M. Cargnello, S. R. Bare, J. Aizenberg, C. M. Friend, A. I. Frenkel  
Nano Lett. 19, 520 (2019)

REVERSE MONTE CARLO AND MOLECULAR DYNAMICS APPROACHES TO EXAFS ANALYSIS

**J. Timoshenko**, A. Kuzmin  
Chapter 5.13 in: X-ray Absorption Spectroscopy and Related Techniques, International Tables for Crystallography, V. 1, IUCR Publisher (**invited**, *in press*).

## 2018

SUBNANOMETER SUBSTRUCTURES IN NANOASSEMBLIES FORMED FROM CLUSTERS UNDER A REACTIVE ATMOSPHERE REVEALED USING MACHINE LEARNING

**J. Timoshenko**, A. Halder, B. Yang, S. Seifert, M. Pellin, S. Vajda, A. I. Frenkel  
J. Phys. Chem. C 122, 21686 (2018)

HIGHLY ACTIVE SUBNANOMETER RH CLUSTERS DERIVED FROM Rh-DOPED SrTiO<sub>3</sub> FOR CO<sub>2</sub> REDUCTION

B. Yan, Q. Wu, J. Cen, **J. Timoshenko**, A. I. Frenkel, D. Su, X. Chen, J. B. Parise, E. A. Stach, A. Orlov, J. G. Chen  
Appl. Catal. B 237, 1003 (2018)

ARTIFICIAL NEURAL NETWORK APPROACH FOR CHARACTERIZING STRUCTURAL TRANSFORMATIONS BY X-RAY ABSORPTION FINE STRUCTURE

**J. Timoshenko**, A. Anspoks, A. Cintins, A. Kuzmin, J. Purans, A. I. Frenkel  
Phys. Rev. Lett 120, 225502 (2018)

STRUCTURAL CHARACTERIZATION OF HETEROGENEOUS Rh-Au NANOPARTICLES FROM A MICROWAVE-ASSISTED SYNTHESIS

Z. Duan, **J. Timoshenko**, P. Kunal, S. House, H. Wan, K. Jarvis, C. Bonifacio, J. C. Yang, R. M. Crooks, A. I. Frenkel, S. Humphrey, G. Henkelman  
Nanoscale 10, 22520 (2018)

INVESTIGATION OF PRECIPITATE IN AN AUSTENITIC ODS STEEL CONTAINING A CARBON-RICH PROCESS CONTROL AGENT

T. Gräning, M. Rieth, A. Kuzmin, A. Anspoks, **J. Timoshenko**, J. Purans, A. Moeslang  
Nucl. Mater. and Energy 15, 237 (2018)

ORIGIN OF PRESSURE-INDUCED METALLIZATION IN  $\text{Cu}_3\text{N}$ : AN X-RAY ABSORPTION SPECTROSCOPY STUDY

A. Kuzmin, A. Anspoks, A. Kalinko, **J. Timoshenko**, L. Nataf, F. Baudelet, and T. Irifune  
Phys. Status Solidi B 255, 1800073 (2018)

GIGAHERTZ SINGLE-ELECTRON PUMPING MEDIATED BY PARASITIC STATES

A. Rossi, J. Klochan, **J. Timoshenko**, F. Hudson, M. Mottonen, S. Rogge, A. Dzurak, V. Kashcheyevs  
Nano Lett. 18, 4141 (2018)

NANOPOROUS COPPER–SILVER ALLOYS BY ADDITIVE-CONTROLLED ELECTRODEPOSITION FOR THE SELECTIVE ELECTROREDUCTION OF  $\text{CO}_2$  TO ETHYLENE AND ETHANOL

T. T. H. Hoang, S. Verma, S. Ma, T. Fister, **J. Timoshenko**, A. I. Frenkel, P. J. A. Kenis, A. A. Gewirth  
J. Am. Chem. Soc. 140, 5791 (2018)

GROWTH OF NANOCATALYST WITH DESIRED CATALYTIC FUNCTIONS BY CONTROLLED DOPING-SEGREGATION OF METAL IN OXIDE

Q. Wu, B. Yan, J. Cen, **J. Timoshenko**, D. Zakharov, X. Chen, H. Xin, S. Yao, J. Parise, A. I. Frenkel, E. A. Stach, J. G. Chen, A. Orlov  
Chem. Mater. 30 (2018), 1585-1592.

CLUSTER ASSEMBLIES PRODUCED BY AGGREGATION OF PREFORMED Ag CLUSTERS IN IONIC LIQUIDS

S. Roese, A. Kononov, **J. Timoshenko**, A. I. Frenkel, H. Hovel  
Langmuir 34, 4811 (2018)

## 2017

SUPERVISED MACHINE LEARNING-BASED DETERMINATION OF THREE-DIMENSIONAL STRUCTURE OF METALLIC NANOPARTICLES

**J. Timoshenko**, D. Lu, Y. Lin, A.I.Frenkel

J. Phys. Chem. Lett. 8, 5091 (2017)

**(highlighted in the virtual issue of The Journal of Physical Chemistry on Machine Learning)**

DETERMINATION OF BIMETALLIC ARCHITECTURES IN NANOMETER-SCALE CATALYSTS BY COMBINING MOLECULAR DYNAMICS SIMULATIONS WITH X-RAY ABSORPTION SPECTROSCOPY

**J. Timoshenko**, K.R.Keller, A.I.Frenkel

J. Chem. Phys. 146, 114201 (2017)

**(JCP editor's selected article)**

PROBING STRUCTURAL RELAXATION IN NANOSIZED CATALYSTS BY COMBINING EXAFS AND REVERSE MONTE CARLO METHODS

**J. Timoshenko**, A.I.Frenkel

Catal. Today 280 (2017) 274.

SIZE DEPENDENT BEHAVIOR OF Fe<sub>3</sub>O<sub>4</sub> CRYSTALS DURING ELECTROCHEMICAL (DE)LITHIATION: AN IN-SITU X-RAY DIFFRACTION, EX-SITU X-RAY ABSORPTION SPECTROSCOPY, TRANSMISSION ELECTRON MICROSCOPY AND THEORETICAL INVESTIGATION

D. C. Bock, C. J. Pelliccione, W. Zhang, **J. Timoshenko**, K. W. Knehr, A. C. West, F. Wang, Y. Li, A. I. Frenkel, E. S. Takeuchi, K. J. Takeuchi, A. C. Marschilok  
Phys. Chem. Chem. Phys. 19, 20867 (2017)

COMPUTATIONALLY ASSISTED STEM AND EXAFS CHARACTERIZATION OF TUNABLE Rh/Au and Rh/Ag BIMETALLIC NANOPARTICLE CATALYSTS

S. D. House, C. S. Bonifacio, **J. Timoshenko**, P. Kunal, H. Wan, Z. Duan, J. C. Yang, A. I. Frenkel, S. M. Humphrey, R. M. Crooks, G. A. Henkelman  
Microsc. Microanal. 23 (Suppl. 1) (2017) 2030-2031.

ROLE OF LEWIS AND BRØNSTED ACIDITY IN METAL CHLORIDE CATALYSIS IN ORGANIC MEDIA: REDUCTIVE ETHERIFICATION OF FURANICS

H. Nguyen, N. Xiao, S. Daniels, N. Marcella, **J. Timoshenko**, A. I. Frenkel, D. Vlachos  
ACS Catalysis 7, 7363 (2017)

STRUCTURAL CHARACTERIZATION OF Rh AND RhAu DENDRIMER – ENCAPSULATED NANOPARTICLES

L. Luo, **J. Timoshenko**, A. Lapp, A. I. Frenkel, R. M. Crooks  
Langmuir 33, 12434 (2017)

THERMAL DISORDER AND CORRELATION EFFECTS IN ANTI-PEROVSKITE-TYPE COPPER NITRIDE

**J. Timoshenko**, A. Anspoks, A. Kalinko, A. Kuzmin  
Acta Mater. 129 (2017) 61-71.

## 2016

IDENTIFICATION OF CARBON-ENCAPSULATED IRON NANOPARTICLES AS ACTIVE SPECIES IN NON-PRECIOUS METAL OXYGEN REDUCTION CATALYSTS

J.A. Varnell, C.M. Edmund, C.E. Schulz, T.T. Fister, R.T. Haasch, **J. Timoshenko**, A.I. Frenkel, A.A. Gewirth.  
Nature Commun. 7, 12582 (2016)

SOLVING LOCAL STRUCTURE AROUND DOPANTS IN METAL NANOPARTICLES WITH AB INITIO MODELING OF X-RAY ABSORPTION NEAR EDGE STRUCTURE,

**J. Timoshenko**, A. Shivhare, R. W. J. Scott, D. Lu, A. I. Frenkel  
Phys. Chem. Chem. Phys.18, 19621 (2016)

A COMBINED THEORETICAL AND EXPERIMENTAL EXAFS STUDY OF THE STRUCTURE AND DYNAMICS OF Au<sub>147</sub> NANOPARTICLES

Z. Duan, Y. Li, **J. Timoshenko**, S. T. Chill, R. M. Anderson, D. F. Yancey, A. I. Frenkel, R. M. Crooks, G. Henkelman  
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EFFECT OF PRESSURE AND TEMPERATURE ON THE LOCAL STRUCTURE AND LATTICE DYNAMICS OF COPPER(II) OXIDE

A. Kuzmin, A. Anspoks, A. Kalinko, A. Rumjancevs, **J. Timoshenko**, L. Nataf, F. Baudelet, T. Irifune

Phys. Procedia 85, 27 (2016).

MOLECULAR DYNAMICS AND REVERSE MONTE CARLO MODELING OF SCHEELITE-TYPE  $AWO_4$  ( $A=Ca, Sr, Ba$ ) W  $L_3$ -EDGE EXAFS SPECTRA

A. Kalinko, A. Bauer, **J. Timoshenko**, A. Kuzmin

Phys. Scr. 91, 114001 (2016)

ATOMISTIC SIMULATIONS OF THE FE K-EDGE EXAFS IN  $FeF_3$  USING MOLECULAR DYNAMICS AND REVERSE MONTE CARLO METHODS

I. Jonane, **J. Timoshenko**, A. Kuzmin

Phys. Scr. 91, 104001 (2016)

LOCAL STRUCTURE OF COPPER NITRIDE REVEALED BY EXAFS SPECTROSCOPY AND REVERSE MONTE CARLO/EVOLUTIONARY ALGORITHM APPROACH

**J. Timoshenko**, A. Anspoks, A. Kalinko, A. Kuzmin

Phys. Scr. 91, 054003 (2016)

STUDY OF COPPER NITRIDE THIN FILM STRUCTURE

A. Kuzmin, A. Kalinko, A. Anspoks, **J. Timoshenko**, R. Kalendarev

Latvian J. Phys. Tech. Sci. 53, 31 (2016)

TEMPERATURE-DEPENDENT EXAFS STUDY OF THE LOCAL STRUCTURE AND LATTICE DYNAMICS IN CUBIC  $Y_2O_3$

I. Jonane, K. Lazdins, **J. Timoshenko**, A. Kuzmin, J. Purans, P. Vladimirov, T. Gräning, J. Hoffmann

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LOCAL DYNAMICS AND PHASE TRANSITION IN QUANTUM PARAELECTRIC  $SrTiO_3$  STUDIED BY Ti K-EDGE X-RAY ABSORPTION SPECTROSCOPY

A. Anspoks, **J. Timoshenko**, J. Purans, F. Rocca, V. Trepakov, A. Dejneka, M. Itoh

J. Phys.: Conf. Ser. 712, 012101 (2016)

PRESSURE-INDUCED INSULATOR-TO-METAL TRANSITION IN  $\alpha$ - $SnWO_4$

A. Kuzmin, A. Anspoks, A. Kalinko, **J. Timoshenko**, R. Kalendarev, L. Nataf, F. Baudelet, T. Irifune, P. Roy,

J. Phys.: Conf. Ser. 712, 012122 (2016)

DISAPPEARANCE OF CORRELATIONS IN THE ATOM MOTION UPON HYDROGEN INTERCALATION INTO  $ReO_3$  LATTICE

**J. Timoshenko**, A. Kuzmin, J. Purans

J. Phys.: Conf. Ser. 712, 012003 (2016)

LOCAL STRUCTURE OF COBALT TUNGSTATE REVEALED BY EXAFS SPECTROSCOPY AND REVERSE MONTE CARLO/EVOLUTIONARY ALGORITHM SIMULATIONS

**J. Timoshenko**, A. Anspoks, A. Kalinko, A. Kuzmin

Z. Phys. Chem. 230, 551 (2016)

THE USE OF X-RAY ABSORPTION SPECTRA FOR VALIDATION OF CLASSICAL FORCE-FIELD MODELS

A. Kuzmin, A. Anspoks, A. Kalinko, **J. Timoshenko**

Z. Phys. Chem. 230, 537 (2016)

**2015**

LOCAL STRUCTURE STUDIES OF Ti FOR SrTi<sup>16</sup>O<sub>3</sub> AND SrTi<sup>18</sup>O<sub>3</sub> BY ADVANCED X-RAY ABSORPTION SPECTROSCOPY DATA ANALYSIS

A. Anspoks, **J. Timoshenko**, D. Bocharov, J. Purans, F. Rocca, A. Sarakovskis, V. Trepakov, A. Dejneka, M. Itoh

Ferroelectrics 485, 42 (2015)

LOCAL STRUCTURE OF MULTIFERROIC MnWO<sub>4</sub> AND Mn<sub>0.7</sub>Co<sub>0.3</sub>WO<sub>4</sub> REVEALED BY THE EVOLUTIONARY ALGORITHM

**J. Timoshenko**, A. Anspoks, A. Kalinko, I. Jonane, A. Kuzmin

Ferroelectrics 483, 68 (2015)

ODS STEEL RAW MATERIAL LOCAL STRUCTURE ANALYSIS USING X-RAY ABSORPTION SPECTROSCOPY

A. Cintins, A. Anspoks, J. Purans, A. Kuzmin, **J. Timoshenko**, P. Vladimirov, T. Graning, J. Hoffmann

IOP Conf. Ser.: Mater. Sci. Eng. 77, 012029 (2015)

EXAFS STUDY OF THE LOCAL STRUCTURE OF CRYSTALLINE AND NANOCRYSTALLINE Y<sub>2</sub>O<sub>3</sub> USING EVOLUTIONARY ALGORITHM METHOD

I. Jonane, **J. Timoshenko**, A. Kuzmin

IOP Conf. Ser.: Mater. Sci. Eng. 77, 012030 (2015)

HIGH-PRESSURE X-RAY ABSORPTION SPECTROSCOPY STUDY OF TIN TUNGSTATES

A. Kuzmin, A. Anspoks, A. Kalinko, **J. Timoshenko**, R. Kalendarev, L. Nataf, F. Baudelet, T. Irifune

Phys. Scripta 90, 094003 (2015)

EXTERNAL PRESSURE AND COMPOSITION EFFECTS ON THE ATOMIC AND ELECTRONIC STRUCTURE OF SnWO<sub>4</sub>

A. Kuzmin, A. Anspoks, A. Kalinko, **J. Timoshenko**, R. Kalendarev

Sol. Energ. Sol. Mat. C 143, 627 (2015)

LOCAL STRUCTURE OF NANOSIZED TUNGSTATES REVEALED BY EVOLUTIONARY ALGORITHM

**J. Timoshenko**, A. Anspoks, A. Kalinko and A. Kuzmin

Phys. Status Solidi A 212, 265 (2015)

**2014**

EXAFS STUDY OF HYDROGEN INTERCALATION INTO  $\text{ReO}_3$  USING THE EVOLUTIONARY ALGORITHM

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(IOP editor's selected article)

LOCAL STRUCTURE AND DYNAMICS OF WURTZITE-TYPE  $\text{ZnO}$  FROM SIMULATION-BASED EXAFS ANALYSIS

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