Janis Timoshenko
LIST OF PUBLICATIONS

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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)

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. (2019, in press)

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, https://doi.org/10.1146/annurev-anchem-061318-114929 (2019)

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. https://doi.org/10.1016/j.radphyschem.2019.04.054 (2019)

SILVER CLUSTERS SHAPE DETERMINATION FROM IN-SITU XANES DATA
J. Timoshenko, S. Roese, H. Hovel, A. I. Frenkel
Rad. Phys. Chem. https://doi.org/10.1016/j.radphyschem.2018.11.003 (2019)

DESIGNING NANOPLATELET 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)

Y. Lin, M. Topsakal, **J. Timoshenko**, D. Lu, S. Yoo, A. I. Frenkel MACHINE-LEARNING ASSISTED DETERMINATION OF COORDINATION NUMBERS OF METALLIC NANOPARTICLES – A BENCHMARK, Chapter in "Experimental Analysis Solutions for Leading Experimental Techniques", World Scientific Publishers, (*accepted*).

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*).

LOCAL STRUCTURE OF A-ATOM IN ABO_3 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. https://doi.org/10.1016/j.radphyschem.2018.11.026 (2019)

INTERPRETATION OF THE Cu K-EDGE EXAFS SPECTRA OF Cu_3N USING AB INITIO MOLECULAR DYNAMICS
D. Bocharov, A. Anspoks, **J. Timoshenko**, A. Kalinko, M. Krack, A. Kuzmin
Rad. Phys. Chem. https://doi.org/10.1016/j.radphyschem.2018.12.020 (2019)

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. https://doi.org/10.1016/j.radphyschem.2018.12.032 (2019)

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 $SrTiO_3$ FOR CO_2 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 Cu_3N: 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 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_3O_4 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_{147} NANOPARTICLES
Z. Duan, Y. Li, **J. Timoshenko**, S. T. Chill, R. M. Anderson, D. F. Yancey, A. I. Frenkel, R. M. Crooks, G. Henkelman
Cat. Sci. Tech. 6, 6879 (2016)
(**invited**).

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
J. Synchrotron Rad. 23, 510 (2016)

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 α-SnWO4

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 $SrTi^{16}O_3$ AND $SrTi^{18}O_3$ 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 $MnWO_4$ AND $Mn_{0.7}Co_{0.3}WO_4$ 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_2O_3 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 $SnWO_4$
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 ReO_3 USING THE EVOLUTIONARY ALGORITHM
J. Timoshenko, A. Kuzmins, J. Purans
J. Phys.: Condens. Mat. 26 (2014) 055401
(**IOP editor's selected article)**

LOCAL STRUCTURE AND DYNAMICS OF WURTZITE-TYPE ZnO FROM SIMULATION-BASED EXAFS ANALYSIS
J. Timoshenko, A. Anspoks, A. Kalinko, A. Kuzmin,
Phys. Status Solidi C 11, 1472 (2014)

TEMPERATURE DEPENDENCE OF THE LOCAL STRUCTURE AND LATTICE DYNAMICS OF WURTZITE-TYPE ZnO
J. Timoshenko, A. Anspoks, A. Kalinko, A. Kuzmin
Acta Mater. 79, 194 (2014)

EXAFS SPECTROSCOPY AND FIRST-PRINCIPLES STUDY OF $SnWO_4$
A. Kuzmin, A. Anspoks, A. Kalinko, **J. Timoshenko**, R. Kalendarev
Phys. Scripta 89, 044005 (2014)

X-RAY ABSORPTION SPECTROSCOPY OF Cu-DOPED WO_3 FILMS FOR USE IN ELECTROCHEMICAL METALLIZATION CELL MEMORY
A. Kuzmin, A. Anspoks, A. Kalinko, **J. Timoshenko**, R. Kalendarev
J. Non-Cryst. Solids 401, 87 (2014)

LOCAL STRUCTURE RELAXATION IN NANOSIZED TUNGSTATES
A. Anspoks, A. Kalinko, **J. Timoshenko**, A. Kuzmin
Solid State Commun. 183, 22 (2014)

ANALYSIS OF EXAFS DATA FROM COPPER TUNGSTATE BY REVERSE MONTE CARLO METHOD
J. Timoshenko, A. Anspoks, A. Kalinko, A. Kuzmin
Phys. Scripta 89, 044006 (2014)

2013

COUNTING STATISTICS FOR ELECTRON CAPTURE IN A DYNAMIC QUANTUM DOT
L. Fricke, M. Wulf, B. Kaestner, V. Kashcheyevs, **J. Timoshenko**, P. Nazarov, F. Hohls, P. Mirovsky, B. Mackrodt, R. Dolata, T. Weimann
Phys. Rev. Lett. 110, 126803 (2013)
(**PRL editor suggested article)**.

, EFFECT OF COBALT DOPING ON THE LOCAL STRUCTURE AND DYNAMICS OF MULTIFERROIC $MnWO_4$ AND $Mn_{0.7}Co_{0.3}WO_4$
A. Kuzmin, A. Anspoks, A. Kalinko, **J. Timoshenko**
J. Phys.: Conf. Ser. 430, 012109 (2013)

AN EFFICIENT IMPLEMENTATION OF THE REVERSE MONTE CARLO METHOD FOR EXAFS ANALYSIS IN CRYSTALLINE MATERIALS,
J. Timoshenko, A. Kuzmin, J. Purans
J. Phys.: Conf. Ser. 430, 012012 (2013)

2012

QUANTUM FLUCTUATIONS AND COHERENCE IN HIGH-PRECISION SINGLE-ELECTRON CAPTURE
V. Kashcheyevs, **J. Timoshenko**
Phys. Rev. Lett. 109, 216801 (2012).

REVERSE MONTE CARLO MODELLING OF THERMAL DISORDER IN CRYSTALLINE MATERIALS FROM EXAFS SPECTRA
J. Timoshenko, A. Kuzmin, J. Purans
Comp. Phys. Commun. 183, 1237 (2012)

2009 - 2011

MOLECULAR DYNAMICS SIMULATIONS OF EXAFS IN GERMANIUM
J. Timoshenko, A. Kuzmin, J. Purans
Cent. Eur. J. Phys. 9, 710 (2011)

PROBING NiO NANOCRYSTALS BY EXAFS SPECTROSCOPY
A. Anspoks, A. Kuzmin, A. Kalinko, **J. Timoshenko**
Solid State Commun. 150, 2270 (2010)

FEMTOMETER ACCURACY EXAFS MEASUREMENTS: ISOTOPIC EFFECT IN THE FIRST, SECOND AND THIRD COORDINATION SHELLS OF GERMANIUM
J. Purans, **J. Timoshenko,** A. Kuzmin, G. Dalba, P. Fornasini, R. Grisenti, N.D. Afify, F. Rocca, S. De Panfilis, I. Ozhogin, S.I. Tiutiunnikov
J. Phys.: Conf. Ser. 190, 012063 (2009)

WAVELET DATA ANALYSIS OF EXAFS SPECTRA
J. Timoshenko, A. Kuzmin
Comp. Phys. Commun. 180, 920 (2009)