

## SERGEY V. USHAKOV

Associate Research Professor  
Center for Materials of the Universe  
School of Molecular Sciences  
Arizona State University  
551 E. University Dr. PSG-106  
Tempe, AZ 85287-1604

Email: sushakov@asu.edu

[ORCID ID 0000-0002-8184-8884](#)

### RESEARCH INTERESTS AND GOALS

- Structure and thermodynamics of oxides, carbides, nitrides at high temperature.
- Application of electromagnetic levitation for ultra high temperature ceramics.
- Application of electrolysis and fractional crystallization of oxide melts for extraterrestrial mining and oxygen production.

### EDUCATION

Postdoctoral Research Associate, Thermochemistry Facility, University of California, Davis CA (with A. Navrotsky)	1999-2003
Ph.D., Mineralogy, St. Petersburg State University, St. Petersburg, Russia (with V.G. Krivovichev)	1994-1998
Short Study, Center for Radioactive Waste Management, University of New Mexico, Albuquerque, NM (with W. Lutze)	1998
Short Study, Department of Earth and Planetary Sciences, University of New Mexico, Albuquerque, NM (with R.C. Ewing)	1996
M.S., Mineralogy, St. Petersburg State University, St. Petersburg, Russia	1989-1994

### EMPLOYMENT

*Associate Research Professor* 2020 - present

Center for Materials of the Universe, School of Molecular Sciences  
Arizona State University, Tempe, AZ

- Experimental research in high temperature thermodynamics and structure of materials relevant to technology, space exploration, and earth and planetary science.
- Advancing experimental techniques and instrumentation for high temperature calorimetry, X-ray and neutron diffraction.
- Integrating experimental thermodynamic and structural data with ab initio models and predictions.

*Staff Research Associate* 2003 - 2020

Thermochemistry laboratory and NEAT ORU,  
University of California Davis, Davis, CA

Co-PI on two collaborative research NSF awards (2015-2018 and 2018-2020)

Research in experimental thermodynamics, instrumentation and technique development:

- High temperature diffraction using synchrotron and neutron sources (PI on 5 proposals).
- Development of drop calorimetry on laser heated aerodynamically levitated samples.
- Application of scanning calorimetry for measurements of surface energies.

- Gas adsorption calorimetry: instrumentation development and application.
- Synthesis of anhydrous nanoparticles by condensation from gas phase.

*Engineer* 1993-1999

Laboratory of Applied Mineralogy,  
Khlopin Radium Institute, St. Petersburg, Russia

Materials synthesis and characterization, reports, and research proposals writing on:

- Chernobyl lavas and hot particles.
- Ceramic formulation for actinide disposal and transmutation.

Fieldwork on existing and prospective nuclear waste disposal sites in Siberia.

## SYNERGETIC ACTIVITIES

- (2023-2024) Guest editor for the special issue of *Materials* on Rare Earth and Actinide Materials
- (2020 -Present) TITAN proposal external team member: cases for ultra-high temperature studies and the design concept of a next-generation hyperbaric electromagnetic levitation system.
- (2020 -Present) Editorial Board Member for MDPI *Materials*
- (2015-2022) Co-organizer of the international research conferences on Structure and Thermodynamic of Oxides (STOHT)
- (2019-2020) Guest editor for the special issue of *Materials* on Thermal Analysis of Materials.
- (2012) Training of students, postdocs, and staff on gas adsorption calorimetry techniques at the University of Free State, Bloemfontein, South Africa.
- Served as a reviewer for NASA, NSF and DOE, South Africa's National Research Foundation proposals, peer reviewer for 18+ journals in the fields of physical chemistry, ceramics, solid state chemistry, and earth and planetary science.

## 3 selected presentations (>90 total)

"Structure and thermodynamics of ceramics above 2000 °C" *13th Asian Thermophysical Properties Conference, ATPC2022*, September 26-30, 2022, Sendai, Japan (*invited*)

"High temperature structure and thermodynamic studies on aerodynamically levitated laser heated oxides." *12th International Workshop on Subsecond Thermophysics*, June 3 - 6, 2019, Cologne, Germany (*invited*)

"Thermal analysis above 1500 °C: state of the art, new results on refractory oxides, and the road ahead." *Gordon Research Conference on High Temperature Materials, Processes & Diagnostics*, July 20-25, 2008, Waterville, ME (*invited*)

## PUBLICATIONS (>90 total, [Google scholar](#) h-index 37, i10-index 71, >4500 citations)

### 3 selected publications (§ undergraduate students advised)

"[Drop-and-catch \(DnC\) calorimetry using aerodynamic levitation and laser heating](#)," S.V. Ushakov, A. Shvarev, T. Alexeev<sup>§</sup>, D. Kapush, A. Navrotsky, *J. Amer. Cer. Soc.*, 100, (2), 754 (2017)

"[Structure and thermal expansion of Lu<sub>2</sub>O<sub>3</sub> and Yb<sub>2</sub>O<sub>3</sub> up to the melting points](#)," A. Pavlik<sup>§</sup>, S.V. Ushakov, A. Navrotsky, C.J. Benmore, R. Weber, *J. Nucl. Mater.*, 495, 385 (2017)

"[Structure and thermal expansion of YSZ and La<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> above 1500 °C from neutron diffraction on levitated samples](#)." S.V. Ushakov, A. Navrotsky, R. Weber, J.C. Neufeind, *J. Amer. Cer. Soc.*, 98, (10), 3381 (2015)

### 3 most cited first author publications ([Google Scholar](#) citation numbers in bold)

["Direct measurements of water adsorption enthalpy on hafnia and zirconia,"](#) S.V. Ushakov, A.

Navrotsky, *Appl. Phys. Lett.*, 87, 164103/1 (2005) (**187 citations**)

["Crystallization in hafnia- and zirconia-based systems,"](#) S.V. Ushakov, A. Navrotsky, Y. Yang, *et al.*

*Phys. Status Solidi B*, 241, 2268-2278 (2004) (**197 citations**)

["Thermochemistry of rare-earth orthophosphates,"](#) S.V. Ushakov, K.B. Helean, A. Navrotsky, L.A.

Boatner, *J. Mater. Res.*, 16, 2623 (2001) (**293 citations**)

### Reviews, book chapters

["Thorium and Rare Earth Monoxides and Related Phases"](#) S.V. Ushakov, Q. Hong, A., D.A. Gilbert, A.

Navrotsky, A. van de Walle, *Materials*, 16(4), 1350 (2023)

["Carbides and Nitrides of Zirconium and Hafnium,"](#) S.V. Ushakov, A. Navrotsky, Q. Hong, A. van de

Walle, *Materials*, 12(17), 2728 (2019)

["Phase transformations in oxides above 2000°C: experimental technique development,"](#) S.V. Ushakov,

P. S. Maram, D. Kapush, et. al , *Adv. Appl. Ceram.*, 117, s82 (2018)

["Experimental approaches to the thermodynamics of ceramics above 1500°C,"](#) S.V. Ushakov and

A. Navrotsky, *J. Am. Ceram. Soc.*, 95 1463-82 (2012)

["Thermodynamics of oxide systems relevant to alternative gate dielectrics,"](#) A. Navrotsky, and

S.V. Ushakov, in: *Materials fundamentals of gate dielectrics*, Eds. by A.A. Demkov and A. Navrotsky,

Kluwer, 57-108, Springer (2005)

### Patents and Records of Invention

"Semiconductor structures and methods of fabricating semiconductor structures comprising hafnium oxide modified with lanthanum, a lanthanide-series metal, or a combination thereof," Z. Yu, J.A. Curless, Y. Liang, A. Navrotsky, S. Ushakov, B-Y Nguyen, A. Demkov *US Patent No. US 7,141,857 B2* issued 11/28/2006

"Method of dosing gases into calorimeter cell" S.V. Ushakov, A. Navrotsky *UC Case No. 2006-026 (2006) patent application was not pursued, instrument constructed and design published*

"Drop-and-catch splat calorimeter for ultra-high-temperature enthalpy measurements" S.V. Ushakov, A. Navrotksy *UC Case No. 2009-396-1 (2009) patent application was not pursued, instrument constructed and design published*

"The design and method of manufacturing of 3D heat flow sensors for high temperature calorimeters" S.V. Ushakov, A. Navrotsky *UC Case No. 2016-660 (2016) patent application was not pursued, the patent rights were released to inventors 08/09/2018*

### Full list of publications

(<sup>§</sup>undergraduate student advised, <sup>†</sup>high school student advised)

"High temperature crystal structure prediction from ab initio molecular dynamics with SLUSCHI" L. Wang, S. V. Ushakov, E. J. Opila, A. Navrotsky, Q.-J. Hong, *Acta Materialia*, 120432 (2024)

"Thermal expansion and enthalpies of phase transformation and fusion of Er<sub>2</sub>O<sub>3</sub> and Tm<sub>2</sub>O<sub>3</sub> from experiment and computation" S.V. Ushakov, Q.-J. Hong, A. Pavlik, III<sup>§</sup>, A. van de Walle, A. Navrotsky,. *Chem. Mater.* 36(9), 4868 (2024)

- "Computationally led high pressure synthesis and experimental thermodynamics of rock salt yttrium monoxide" B.L. Brugman, Y. Han, L.J. Leinbach, K. Leinenweber, A. van de Walle, S.V. Ushakov, Q.-J. Hong, A. Navrotsky, *Chem. Mater.* 36(1), 332 (2024)
- "Thorium and rare earth monoxides and related phases" S.V. Ushakov, Q. Hong, A., D.A. Gilbert, A. Navrotsky, A. van de Walle, *Materials* 16(4), 1350 (2023)
- "Structure and thermodynamics of oxides/carbides/nitrides/borides at high temperatures" Q. Hong, S.V. Ushakov, K. Lilova, A. Navrotsky, S.J. McCormack, *Am. Ceram. Soc. Bull.* 102 (2), 28 (2023)
- "Impact of prolonged heating on the color and crystallinity of bone" G. Gallo, S.V. Ushakov, A. Navrotsky, M.C. Stahlschmidt, *Archaeol. Anthropol. Sci.* 15(9), 143 (2023)
- "Melting temperature prediction using a graph neural network model: From ancient minerals to new materials," Q. Hong, S.V. Ushakov, A. van de Walle, A. Navrotsky, *PNAS* 119 (36), e2209630119 (2022)
- "Integrating computational and experimental thermodynamics of refractory materials at high temperature," Q. Hong, A. van de Walle, S.V. Ushakov, A. Navrotsky, *Calphad* 79, 102500 (2022)
- "Energetics of reactions between ceramic coating materials and their binary oxide components with silicate melts" G. Costa, B.J. Harder, N.P. Bansal, J.L. Stokes, K. Lilova, T. Subramani, S.V. Ushakov, K.J. Meisner, A. Navrotsky, *J. Am. Ceram. Soc.* 105 (12), 7795 (2022)
- "Multi-extreme conditions at the Second Target Station" B. Haberl, D.G. Quirinale, C.W. Li, G.E. Granroth, H. Nojiri, M.E. Donnelly, S.V. Ushakov, R. Boehler, B.L. Winn, *Rev. Sci. Instr.* 93 (8), 083907
- "Measurements of Density of Liquid Oxides with an Aero-Acoustic Levitator," S.V. Ushakov, J. Niessen, D.G. Quirinale, R. Prieler, A. Navrotsky, R. Telle, *Materials* 14, (4), 822 (2021)
- "Characterization of structural changes in modern and archaeological burnt bone: Implications for differential preservation bias," G. Gallo, M. Fyhrie<sup>§</sup>, C. Paine, S.V. Ushakov, M. Izuho, B. Gunchinsuren, N. Zwyns, A. Navrotsky, *PLoS One*, 16, (7), e0254529 (2021)
- "A simple method for computing the formation free energies of metal oxides," H. Chen, Q. Hong, S. Ushakov, A. Navrotsky, A. van de Walle, *Computational Materials Science*, 198, 110692 (2021)
- "Thermochemistry and phase stability of the polymorphs of yttrium tantalate, YTaO<sub>4</sub>," M. Lepple, S.V. Ushakov, K. Lilova, C.A. Macauley, A.N. Fernandez, C.G. Levi, A. Navrotsky, *J. Eur. Cer. Soc.* 41(2), 1629-38 (2021)
- "Thermal Analysis of High Entropy Rare Earth Oxides," S.V. Ushakov, S. Hayun, W. Gong, A. Navrotsky *Materials* 13 (14), 3141 (2020)
- "Thermodynamic assessment of BaO–Ln<sub>2</sub>O<sub>3</sub> (Ln = La, Pr, Eu, Gd, Er) systems," W. Gong, Y. Liu, Y. Xie, Z. Zhao, S.V. Ushakov, A. Navrotsky, *J. Am. Ceram. Soc.* 103 (6), 3896-904 (2020)
- "Carbides and Nitrides of Zirconium and Hafnium," S.V. Ushakov, A. Navrotsky, Q.-J. Hong, and A. van de Walle, *Materials*, 12[17] 2728 (2019)
- "Synthesis, Crystal Structure and Enthalpies of Formation of Churchite-type REPO<sub>4</sub>·2H<sub>2</sub>O (RE = Gd to Lu) Materials," T. Subramani, M.R. Rafiuddin, A. Shelyug, S.V. Ushakov, A. Mesbah, N. Clavier, D. Qin, S. Szenknect, E. Elkaim, N. Dacheux, and A. Navrotsky, *Crystal Growth & Design*, 19[8] 4641-9 (2019)
- "Polymer-Derived Ultra-High Temperature Ceramics (UHTCs) and Related Materials," E. Ionescu, S. Bernard, R. Lucas, P. Kroll, S. Ushakov, A. Navrotsky, R. Riedel, *Adv. Eng. Mater.* 1 (8), 1900269 (2019)
- "In-situ determination of the HfO<sub>2</sub>–Ta<sub>2</sub>O<sub>5</sub>-temperature phase diagram up to 3000°C," S.J. McCormack, K.-P. Tseng, R.J.K. Weber, D. Kapush, S.V. Ushakov, A. Navrotsky, and W. M. Kriven, *J. Am. Ceram. Soc.*, 102[8] 4848-61 (2019)
- "Energetics of hydration on uranium oxide and peroxide surfaces," X. Guo, D. Wu, S.V. Ushakov, T. Shvareva, H. Xu, and A. Navrotsky, *J. Mat. Res.* 1-7 (2019)
- "Energetics of melting of Yb<sub>2</sub>O<sub>3</sub> and Lu<sub>2</sub>O<sub>3</sub> from drop and catch calorimetry and first principles computations," M. Fyhrie<sup>§</sup>, Q.-J. Hong, D. Kapush, S.V. Ushakov, H. Liu, A. van de Walle, and A. Navrotsky, *J. Chem. Thermodyn.*, 132 405-10 (2019)

- "Thermodynamics of reaction between gas-turbine ceramic coatings and ingested CMAS corrodents," G. Costa, B. J. Harder, V. L. Wiesner, D. Zhu, N. Bansal, K. N. Lee, N. S. Jacobson, D. Kapush, S.V. Ushakov, and A. Navrotsky, *J. Am. Ceram. Soc.* 102[5] 2948-64 (2019)
- "Phase transformations in oxides above 2000°C: experimental technique development," S.V. Ushakov, P. S. Maram, D. Kapush, A. J. Pavlik<sup>§</sup>, III, M. Fyhrie<sup>§</sup>, L. C. Gallington, C.J. Benmore, R. Weber, J.C. Neufeind, J.W. McMurray, and A. Navrotsky, *Adv. Appl. Ceram.*, 117[sup1] s82-9 (2018)
- "Size driven thermodynamic crossovers in phase stability in zirconia and hafnia," G. Sharma, S.V. Ushakov, and A. Navrotsky, *J. Am. Ceram. Soc.*, 101[1] 31-35 (2018)
- "Probing disorder in pyrochlore oxides using in situ synchrotron diffraction from levitated solids-A thermodynamic perspective," P. S. Maram, S.V. Ushakov, R. J. K. Weber, C. J. Benmore, and A. Navrotsky, *Sci. Rep.*, 8[1] 1-11 (2018)
- "Combined computational and experimental investigation of high temperature thermodynamics and structure of cubic ZrO<sub>2</sub> and HfO<sub>2</sub>," Q.-J. Hong, S.V. Ushakov, D. Kapush, C. J. Benmore, R. J.K. Weber, A. van de Walle, and A. Navrotsky, *Scientific Reports*, 8[1] 14962 (2018)
- "Thermochemistry of BaSm<sub>2</sub>O<sub>4</sub> and thermodynamic assessment of the BaO-Sm<sub>2</sub>O<sub>3</sub> system," W. Gong, S.V. Ushakov, C. Agca, and A. Navrotsky, *J. Am. Ceram. Soc.*, 101[12] 5827-35 (2018)
- "Calorimetric Measurements of Surface Energy of Amorphous HfO<sub>2</sub> Nanoparticles Produced by Gas Phase Condensation," G. Sharma, S.V. Ushakov, H. Li, R. H. R. Castro, and A. Navrotsky, *J. Phys. Chem. C*, 121[19] 10392-97 (2017)
- "A combined experimental and theoretical study of enthalpy of phase transition and fusion of yttria above 2000°C using "drop-n-catch" calorimetry and first-principles calculation," D. Kapush, S. Ushakov, A. Navrotsky, Q.-J. Hong, H. Liu, and A. van de Walle, *Acta Materialia*, 124 204-09 (2017)
- "Drop-and-catch (DnC) calorimetry using aerodynamic levitation and laser heating," S.V. Ushakov, A. Shvarev, T. Alexeev<sup>§</sup>, D. Kapush, and A. Navrotsky, *J. Am. Ceram. Soc.*, 100[2] 754-60 (2017)
- "Hot matters - experimental methods for high-temperature property measurement," A. Navrotsky and S.V. Ushakov, *Am. Ceram. Soc. Bull.*, 96[2] 22-28 (2017)
- "Solid-liquid phase equilibria of Fe-Cr-Al alloys and spinels," J. W. McMurray, R. Hu<sup>§</sup>, S.V. Ushakov, D. Shin, B. A. Pint, K. A. Terrani, and A. Navrotsky, *J. Nucl. Mater.*, 492 128-33 (2017)
- "Structure and thermal expansion of Lu<sub>2</sub>O<sub>3</sub> and Yb<sub>2</sub>O<sub>3</sub> up to the melting points," A. Pavlik<sup>§</sup>, S.V. Ushakov, A. Navrotsky, C. J. Benmore, and R. J. K. Weber, *J. Nucl. Mater.*, 495, 385-91 (2017)
- "The Structure of Liquid and Amorphous Hafnia," L. Gallington, Y. Ghadar, L. Skinner, J. Weber, S. Ushakov, A. Navrotsky, A. Vazquez-Mayagoitia, J. Neufeind, M. Stan, J. Low, and C. Benmore, *Materials*, 10[11] 1290 (2017)
- "Tunable Low Density Palladium Nanowire Foams," D. A. Gilbert, E. C. Burks, S.V. Ushakov, P. Abellan, I. Arslan, T. E. Felter, A. Navrotsky, and K. Liu, *Chem. Mater.*, 29[22] 9814-18 (2017)
- "Phase transformations and indications for acoustic mode softening in Tb-Gd orthophosphate," O. Tschauner, S.V. Ushakov, A. Navrotsky, and L. A. Boatner, *Journal of Physics: Condensed Matter*, 28[3] 035403 (2016)
- "Combined computational and experimental investigation of the refractory properties of La<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub>," Q.-J. Hong, S.V. Ushakov, A. Navrotsky, and A. van de Walle, *Acta Mater.*, 84 275-82 (2015)
- "In Situ Diffraction from Levitated Solids Under Extreme Conditions-Structure and Thermal Expansion in the Eu<sub>2</sub>O<sub>3</sub>-ZrO<sub>2</sub> System," P. S. Maram, S.V. Ushakov, R. J.K. Weber, C. J. Benmore, and A. Navrotsky, *J. Am. Ceram. Soc.*, 98[4] 1292-99 (2015)
- "Structure and Thermal Expansion of YSZ and La<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> Above 1500°C from Neutron Diffraction on Levitated Samples," S.V. Ushakov, A. Navrotsky, R. J. K. Weber, J.C. Neufeind, *J. Am. Ceram. Soc.*, 98[10] 3381-88 (2015)

- "Thermodynamic complexity of carbon capture in alkylamine-functionalized metal-organic frameworks," D. Wu, T. M. McDonald, Z. Quan, S. V. Ushakov, P. Zhang, J. R. Long, and A. Navrotsky, *J. Mater. Chem. A*, 3[8] 4248-54 (2015)
- "Thermodynamics of formation of coffinite,  $\text{USiO}_4$ ," X. Guo, S. Szenknect, A. Mesbah, N. Clavier, C. Poinsot, S.V. Ushakov, H. Curtius, D. Bosbach, R. C. Ewing, and P. C. Burns, *Proc. of the National Academy of Sciences*, 112[21] 6551-55 (2015)
- "Thermodynamics of solid phases containing rare earth oxides," A. Navrotsky, W. Lee, A. Mielewczik-Gryn, S.V. Ushakov, A. Anderko, H. Wu, and R. E. Rimman, *J. Chem. Therm.*, 88 126-41 (2015)
- "Direct Measurement of Fusion Enthalpy of  $\text{LaAlO}_3$  and Comparison of Energetics of Melt, Glass, and Amorphous Thin Films," S.V. Ushakov and A. Navrotsky, *J. Am. Ceram. Soc.*, 97[5] 1589-94 (2014)
- "Energetics of  $\text{CO}_2$  and  $\text{H}_2\text{O}$  Adsorption on Zinc Oxide," D. Gouvêa, S.V. Ushakov, and A. Navrotsky, *Langmuir*, 30[30] 9091-97 (2014)
- "Energetics of metastudtite and implications for nuclear waste alteration," X. Guo, S.V. Ushakov, S. Labs, H. Curtius, D. Bosbach, and A. Navrotsky, *Proc. Natl. Acad. Sci. U. S. A.*, 111[50] 17737-42 (2014)
- "Ultra-high temperature oxidation of a hafnium carbide-based solid solution ceramic composite," D. W. Lipke, S.V. Ushakov, A. Navrotsky, and W. P. Hoffman, *Corros. Sci.*, 80 402-07 (2014)
- "Amorphous Alumina Nanoparticles: Structure, Surface Energy and Thermodynamic Phase Stability," A. H. Tavakoli, P. S. Maram, S. J. Widgeon, J. Rufner, K. van Benthem, S.V. Ushakov, S. Sen, and A. Navrotsky, *J. Phys. Chem. C*, 117 17123-30 (2013)
- "Direct Calorimetric Measurement of Enthalpy of Adsorption of Carbon Dioxide on CD-MOF-2, a Green Metal-Organic Framework," D. Wu, J. J. Gassensmith, D. Gouvêa, S.V. Ushakov, J. F. Stoddart, and A. Navrotsky, *J. Am. Chem. Soc.*, 135[8] 6790-3 (2013)
- "Noble Gas Adsorption in Copper Trimesate, HKUST-1: An Experimental and Computational Study," Z. Hulvey, K. V. Lawler, Z. Qiao, J. Zhou, D. Fairen-Jimenez, R. Q. Snurr, S.V. Ushakov, A. Navrotsky, C. M. Brown, and P. M. Forster, *J. Phys. Chem. C*, 117[39] 20116-26 (2013)
- "Experimental approaches to the thermodynamics of ceramics above 1500°C," S.V. Ushakov and A. Navrotsky, *J. Am. Ceram. Soc.*, 95[5] 1463-82 (2012)
- "Fluorite-pyrochlore transformation in  $\text{Eu}_2\text{Zr}_2\text{O}_7$ -direct calorimetric measurement of phase transition, formation and surface enthalpies," M. P. Saradhi, S.V. Ushakov, and A. Navrotsky, *RSC Adv.*, 2 3328-34 (2012)
- "Yttria-stabilized hafnia: thermochemistry of formation and hydration of nanoparticles," W. Zhou, S.V. Ushakov, and A. Navrotsky, *J. Mater. Res.*, 27[7], 022-28 (2012)
- "Yttria-stabilized zirconia crystallization in  $\text{Al}_2\text{O}_3/\text{YSZ}$  multilayers," N. Kemik, S.V. Ushakov, M. Gu, N. Schichtel, C. Korte, N. D. Browning, Y. Takamura, and A. Navrotsky, *J. Mater. Res.*, 27 939-43 (2012)
- "Direct measurements of fusion and phase transition enthalpies in lanthanum oxide," S.V. Ushakov and A. Navrotsky, *J. Mater. Res.*, 26 845-47 (2011)
- "Application of scanning calorimetry to estimate soil organic matter loss after fires," S.V. Ushakov, D. Nag†, and A. Navrotsky, *J. Therm. Anal. Calorim.*, 104[1] 351-56 (2011)
- "Yttrium substitution in  $\text{MTiO}_3$  ( $\text{M} = \text{Ca}, \text{Sr}, \text{Ba}$  and  $\text{Ca}+\text{Sr}+\text{Ba}$ ) perovskites and implication for incorporation of fission products into ceramic waste forms," N. U. Navi, G. Kimmel, J. Zabicky, S.V. Ushakov, R. Z. Shneck, M. H. Mintz, and A. Navrotsky, *J. Am. Ceram. Soc.*, 94[9] 3112-16 (2011)
- "Direct measurement of surface energy of  $\text{CeO}_2$  by differential scanning calorimetry," S. Hayun, S.V. Ushakov, and A. Navrotsky, *J. Am. Ceram. Soc.*, 94[11] 3679-82 (2011)
- "Experimental Methodologies for Assessing the Surface Energy of Highly Hygroscopic Materials: The Case of Nanocrystalline Magnesia," S. Hayun, T. Tran, S.V. Ushakov, A. M. Thron, B. K. van, A. Navrotsky, and R. H. R. Castro, *J. Phys. Chem. C*, 115[48] 23929-35 (2011)

- "Hafnia: energetics of thin films and nanoparticles," W. Zhou, S.V. Ushakov, T. Wang, J. G. Ekerdt, A. A. Demkov, and A. Navrotsky, *J. Appl. Phys.*, 107[12] 123514/1-7 (2010)
- "Synthesis and calorimetric studies of oxide multilayer systems: Solid oxide fuel cell cathode and electrolyte materials," N. Kemik, S.V. Ushakov, N. Schichtel, C. Korte, Y. Takamura, and A. Navrotsky, *J. Vac. Sci. Technol. B*, 28[4] C5A1-5 (2010)
- "Calorimetric Measurement of Surface and Interface Enthalpies of Yttria-Stabilized Zirconia (YSZ)," G. C. C. Costa, S.V. Ushakov, R. H. R. Castro, A. Navrotsky, and R. Muccillo, *Chem. Mater.*, 22[9] 2937-45 (2010)
- "Thermochemistry of lanthanum zirconate pyrochlore," A. V. Radha, S.V. Ushakov, and A. Navrotsky, *J. Mater. Res.*, 24[11] 3350-57 (2009)
- "Monoclinic to tetragonal transformations in hafnia and zirconia: A combined calorimetric and density functional study," X. Luo, W. Zhou, S.V. Ushakov, A. Navrotsky, and A. A. Demkov, *Phys. Rev. B: Condens. Matter Mater. Phys.*, 80[13] 134119/1-13 (2009)
- "Fluorite and pyrochlore phases in the  $\text{HfO}_2\text{-La}_2\text{O}_3\text{-Gd}_2\text{O}_3$  systems: characterization and calorimetric study of samples quenched from melts formed by laser heating and aerodynamic levitation," S.V. Ushakov, A. Navrotsky, and J. A. Tangeman, *Mater. Res. Soc. Symp. Proc.*, 1122E, 1122-O01-07 (2008)
- "Thermochemistry of nanoparticles on a substrate: zinc oxide on amorphous silica," T. Y. Shvareva, S.V. Ushakov, A. Navrotsky, J. A. Libera, and J. W. Elam, *J. Mater. Res.*, 23[7] 1907-15 (2008)
- "Surface enthalpy, enthalpy of water adsorption, and phase stability in nanocrystalline monoclinic zirconia," A. V. Radha, O. Bomati-Miguel, S.V. Ushakov, A. Navrotsky, and P. Tartaj, *J. Am. Ceram. Soc.*, 92[1] 133-40 (2009)
- "Energetics of  $\text{La}_2\text{O}_3\text{-HfO}_2\text{-SiO}_2$  glasses," R. M. Morcos, J. Tangeman, S. Ushakov, and A. Navrotsky, *J. Am. Ceram. Soc.*, 91[4] 1088-94 (2008)
- "Thermochemistry of  $\text{A}_2\text{M}_3\text{O}_{12}$  negative thermal expansion materials," T. Varga, J. L. Moats, S.V. Ushakov, and A. Navrotsky, *J. Mater. Res.*, 22[9] 2512-21 (2007)
- "Energetics of defect fluorite and pyrochlore phases in lanthanum and gadolinium hafnates," S.V. Ushakov, A. Navrotsky, J. A. Tangeman, and K. B. Helean, *J. Am. Ceram. Soc.*, 90[4] 1171-76 (2007)
- "Surface Energy and Thermodynamic Stability of  $\gamma$ -Alumina: Effect of Dopants and Water," R. H. R. Castro, S.V. Ushakov, L. Gengembre, D. Gouvea, and A. Navrotsky, *Chem. Mater.*, 18 1867-72 (2006)
- "Direct measurements of water adsorption enthalpy on hafnia and zirconia," S.V. Ushakov and A. Navrotsky, *Appl. Phys. Lett.*, 87 164103/1-03/3 (2005)
- "Energy crossovers in nanocrystalline zirconia," M. W. Pitcher, S.V. Ushakov, A. Navrotsky, B. F. Woodfield, G. Li, J. Boerio-Goates, and B. M. Tissue, *J. Am. Ceram. Soc.*, 88 160-67 (2005)
- "Thermodynamics of oxide systems relevant to alternative gate dielectrics," A. Navrotsky and S.V. Ushakov, pp. 57-108. in Materials Fundamentals of Gate Dielectrics Edited by A. Demkov and A. Navrotsky, Springer, Netherlands, 2005.
- "Formation enthalpy of  $\text{ThSiO}_4$  and enthalpy of the thorite  $\rightarrow$  huttonite phase transition," L. Mazeina, S.V. Ushakov, A. Navrotsky, and L.A. Boatner, *Geochim. Cosmochim. Acta*, 69[19] 4675-83 (2005)
- "Crystallization in hafnia- and zirconia-based systems," S.V. Ushakov, A. Navrotsky, Y. Yang, S. Stemmer, K. Kukli, M. Ritala, M. A. Leskelae, P. Fejes, A. Demkov, C. Wang, B. Y. Nguyen, D. Triyoso, and P. Tobin, *Phys. Status Solidi B*, 241 2268-78 (2004)
- "Thermochemistry of the alkali rare-earth double phosphates,  $\text{A}_3\text{RE}(\text{PO}_4)_2$ ," S.V. Ushakov, A. Navrotsky, J. M. Farmer, and L.A. Boatner, *J. Mater. Res.*, 19[7] 2165-75 (2004)
- "Effect of La and Y on crystallization temperatures of hafnia and zirconia," S.V. Ushakov, C.E. Brown<sup>§</sup>, and A. Navrotsky, *J. Mater. Res.*, 19[3] 693-96 (2004)

- "Formation enthalpies of rare earth titanate pyrochlores," K. B. Helean, S.V. Ushakov, C.E. Brown<sup>§</sup>, A. Navrotsky, J. Lian, R. C. Ewing, J. M. Farmer, and L.A. Boatner, *J. Solid State Chem.*, 177[6] 1858-66 (2004)
- "Thermal analyses of bulk amorphous oxides and silicates of zirconium and hafnium," S.V. Ushakov, C. E. Brown<sup>§</sup>, A. Navrotsky, A. Demkov, C. Wang, and B.Y. Nguyen, *Mater. Res. Soc. Symp. Proc.*, 745 3-8 (2003)
- "Formation enthalpies of tetravalent lanthanide perovskites by high temperature oxide melt solution calorimetry," S.V. Ushakov, J. Cheng, A. Navrotsky, J.R. Wu, and S.M. Haile, *Mater. Res. Soc. Symp. Proc.*, 718 71-76 (2002)
- "Thermochemistry of rare-earth orthophosphates," S.V. Ushakov, K.B. Helean, A. Navrotsky, and L.A. Boatner, *J. Mater. Res.*, 16[9] 2623-33 (2001)
- "Formation energetics of ceramic phases related to surplus plutonium disposal," R.L. Putnam, U.F. Gallegos, A. Navrotsky, K.B. Helean, S.V. Ushakov, B.F. Woodfield, J. Boerio-Goates, B.B. Ebbinghaus, and M. A. Williamson, *Ceram. Trans.*, 119, 147-58 (2001)
- "Solid solutions of Ce, U, and Th in zircon," S.V. Ushakov, W. Gong, M.M. Yagovkina, K.B. Helean, W. Lutze, and R.C. Ewing, *Ceram. Trans.*, 93, 357-63 (1999)
- "Synthesis of Ce-doped zircon by a sol-gel process," S.V. Ushakov, B.E. Burakov, V.M. Garbuzov, E.B. Anderson, E.E. Strykanova, M.M. Yagovkina, K.B. Helean, Y.X. Guo, R.C. Ewing, and W. Lutze, *Mater. Res. Soc. Symp. Proc.*, 506, 281-88 (1998)
- "Interaction of UO<sub>2</sub> and Zircaloy during the Chernobyl accident," S.V. Ushakov, B.E. Burakov, S.I. Shabalev, and E. B. Anderson, *Mater. Res. Soc. Symp. Proc.*, 465, 1313-18 (1997)
- "Mineralogical and microtextural characterization of "gel-zircon" from the Manibay uranium mine Kazakhstan," K. B. Helean, B. E. Burakov, E. B. Anderson, E. E. Strykanova, S.V. Ushakov, and R. C. Ewing, *Mater. Res. Soc. Symp. Proc.*, 465, 1219-26 (1997)
- "The behavior of nuclear fuel in first days of the Chernobyl accident," B. E. Burakov, E. B. Anderson, S. I. Shabalev, E. E. Strykanova, S.V. Ushakov, M. Trotabas, J. Y. Blanc, P. Winter, and J. Duco, *Mater. Res. Soc. Symp. Proc.*, 465, 1297-308 (1997)
- "Synthesis of zircon for immobilization of actinides," B. E. Burakov, E. B. Anderson, V. S. Rovsha, S.V. Ushakov, R. C. Ewing, W. Lutze, and W. J. Weber, *Mater. Res. Soc. Symp. Proc.*, 412, 33-9 (1996)