

# CURRICULUM VITAE

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## WORK EXPERIENCE

- 03/2022 - present Marie Curie postdoctoral fellow, German Aerospace Center (DLR), Stuttgart, Germany
- 03/2022 - present Guest researcher/Marie Curie fellow, Delft University of Technology, Delft, Netherlands
- 05/2018 – 03/2022 Postdoctoral researcher, Eindhoven University of Technology, Eindhoven, Netherlands
- 10/2020 - 12/2020 Visiting scientist, Friedrich-Alexander-Universität Erlangen-Nürnberg, Computer Chemistry Center, Erlangen, Germany
- 03/2017 - 04/2017 Visiting scholar (WRHI), Tokyo Institute of Technology, Tokyo, Japan
- 09/2015 - 04/2018 Assistant lecturer at Novosibirsk State University, Novosibirsk, Russia

## EDUCATION AND TRAINING

- 10/2012 - 06/2016 PhD in Physical Chemistry, 2016, Boreskov Institute of Catalysis, Novosibirsk, Russia
- 09/2007 - 06/2012 Specialist in Chemistry, *summa cum laude*, GPA 5.0, Novosibirsk State University

## RESEARCH EXPERTISE AND TECHNICAL SKILLS

### Areas of expertise

- Thermal energy storage and transformation
- Sorption and thermochemical cycles and systems
- Preparation and characterization of composites and nanoparticles
- Solid state kinetics and mechanisms of solid-state transformations
- Chemical thermodynamics and calorimetry
- Atomic scale simulations (DFT, MD) and characterization of electronic structure

### Software and programming

- Python
- Origin
- MATLAB

### Experimental methods

- Thermal analysis (TGA, DSC, DVS)
- X-ray diffraction analysis
- Texture characterization
- Vibrational and UV-vis spectroscopy
- NMR imaging and relaxometry
- Electron microscopy (SEM, HRTEM)

### Other skills

- Mentoring students
- Preparation and publishing of papers in scientific journals
- Writing scientific proposals

### Languages

- English (C1, CAE certificate)
- German (basic)
- Dutch (basic)
- Russian (native)

## PUBLICATIONS

- Papers in refereed journals: 18, 1 book chapter
- Communications to scientific meetings (oral): 19

Reviewer: Advanced Materials, Applied Energy, Energy Conversion and Management, etc.

### List of journal papers:

1. Eberbach, M., Huinink, H., **Shkatulov, A.**, Fischer, H., Adan O.C.G The Effect of Nanoconfinement on Deliquescence of CuCl<sub>2</sub> Is Stronger than on Hydration, *Cryst. Growth Des.* 2023, 23, 3, 1343–1354.
2. Houben J., **Shkatulov A.**, Huinink H., Fischer H., Adan, O.C.G. Caesium doping accelerates the hydration rate of potassium carbonate in thermal energy storage, *Solar Energy Materials and Solar Cells*, 2023, 251, 112116
3. **Shkatulov A.**, Becit B, Zahn D. Molecular Dynamics Simulations of Nitrate/MgO Interfaces and Understanding Metastability of Thermochemical Materials. *ACS Omega* 2022;7:16371–9.
4. **Shkatulov, A.**; Miura, H;Kim, S. T.;Zamengo, M.;Harada, T.;Takasu, H.;Kato, Y.;Aristov, Y. Thermochemical storage of medium-temperature heat using MgO promoted with eutectic ternary mixture LiNO<sub>3</sub>-NaNO<sub>3</sub>-KNO<sub>3</sub>, *Journal of Energy Storage*, 2022, 51, 104409
5. Solovyeva MV, **Shkatulov AI**, Gordeeva LG, Fedorova EA, Krieger TA, Aristov YI. Water Vapor Adsorption on CAU-10-X: Effect of Functional Groups on Adsorption Equilibrium and Mechanisms. *Langmuir* 2021;37:693–702.
6. **Shkatulov, A.I.**, Joosten, R., Fischer, H., Huinink, H. Core-shell encapsulation of salt hydrates into mesoporous silica shells for thermochemical energy storage, *ACS Appl. Energy Mater.* 2020, 3, 7, 6860–6869.
7. **Shkatulov A. I.**, Gordeeva L.G., Girnik I.S., Huinink H.P., Aristov Y. Novel adsorption method for moisture and heat recuperation in ventilation: Composites “LiCl/matrix” tailored for cold climate, *Energy* (2020), 117595
8. **Shkatulov, A.I.**, Houben, J., Fischer, H., Huinink, H.P. Stabilization of K<sub>2</sub>CO<sub>3</sub> in vermiculite for thermochemical energy storage (2020) *Renewable Energy*, 150, pp. 990-1000.
9. Kim, S.T., Miura, H., Takasu, H., Kato, Y., **Shkatulov, A.**, Aristov, Y. Adapting the MgO-CO<sub>2</sub> working pair for thermochemical energy storage by doping with salts: Effect of the (LIK)NO<sub>3</sub> content (2019) *Energies*, 12 (11), art. no. 2262, .
10. **Shkatulov, A. I.**, Takasu, H., Kato, Y., Aristov, Y. Thermochemical energy storage by LiNO<sub>3</sub>-doped Mg(OH)<sub>2</sub> : Rehydration study (2019) *Journal of Energy Storage*, 22, pp. 302-310.
11. **Shkatulov, A.I.**, Kim, S.T., Miura, H., Kato, Y., Aristov, Y.I. Adapting the MgO-CO<sub>2</sub> working pair for thermochemical energy storage by doping with salts (2019) *Energy Conversion and Management*, 185, pp. 473-481.
12. Bakovets, V.V., Sotnikov, A.V., Agazhanov, A.S., Stankus, S.V., Korotaev, E.V., Pishchur, D.P., **Shkatulov, A.I.** Some features of thermophysical properties of  $\gamma$ -Gd<sub>2</sub>S<sub>3</sub> ceramics based on real structure (2018) *Journal of the American Ceramic Society*, 101 (10), pp. 4773-4782.
13. **Shkatulov, A.I.**, Aristov, Y. Thermochemical Energy Storage using LiNO<sub>3</sub>-Doped Mg(OH)<sub>2</sub>: A Dehydration Study (2018) *Energy Technology*, 6 (9), pp. 1844-1851.
14. Tokarev, M.M., Gordeeva, L.G., **Shkatulov, A.I.**, Aristov, Y.I. Testing the lab-scale “Heat from Cold” prototype with the “LiCl/silica – methanol” working pair (2018) *Energy Conversion and Management*, 159, pp. 213-220.
15. **Shkatulov, A.**, Aristov, Y. Calcium hydroxide doped by KNO<sub>3</sub> as a promising candidate for thermochemical storage of solar heat (2017) *RSC Advances*, 7 (68), pp. 42929-42939.

16. **Shkatulov, A.**, Aristov, Y. Modification of magnesium and calcium hydroxides with salts: An efficient way to advanced materials for storage of middle-temperature heat (2015) *Energy*, 85, pp. 667-676.
17. **Shkatulov, A.**, Krieger, T., Zaikovskii, V., Chesalov, Y., Aristov, Y. Doping magnesium hydroxide with sodium nitrate: A new approach to tune the dehydration reactivity of heat-storage materials (2014) *ACS Applied Materials and Interfaces*, 6 (22), pp. 19966-19977.
18. **Shkatulov, A.**, Ryu, J., Kato, Y., Aristov, Y. Composite material "Mg(OH)<sub>2</sub>/vermiculite": A promising new candidate for storage of middle temperature heat (2012) *Energy*, 44 (1), pp. 1028-1034.

**Book chapters:**

1. Gordeeva L.G., **Shkatulov A.I.**, Aristov Yu. I. Closed sorption systems in: Encyclopedia of Energy Storage, Volume 1, 2022, Pages 542-558, Cabeza L. F. ed., Elsevier.

**List of oral communications to scientific meetings:**

1. **Shkatulov, A.I.**, Huinink H.P. Salt hydrates for low- and ultralow-temperature heat transformation, International Symposium on Innovative Materials and Processes in Energy Systems, Barcelona, 25-27 October 2022
2. **Shkatulov, A.I.**, Genç, A.E., Tranca I.C. Exploring structure-property relationships for hydration and carbonation of metal oxides for thermochemical energy storage, E-MRS Fall meeting 2022, Wawrsaw, 19-21 September 2022
3. **Shkatulov A.I.**, Tranca I., Huinink H., Machine learning aided screening of new salt hydrates for thermochemical energy storage, NWO Chains conference, 6-8 December 2021.
4. **Shkatulov A. I.**, Huinink, H. Core-shell composites for thermochemical energy storage with high storage density, Materials Science and Engineering Congress (MSE 2020), 22-25 September 2020.
5. **Shkatulov A. I.**, Solovyeva M. V., Gordeeva L.G., Aristov Y.I. Water vapor adsorption on CAU-10-X: effect of functional groups on adsorption equilibrium and mechanisms, CMD2020GEFES, 31 August – 04 September 2020
6. **Shkatulov, A.I.**, Huinink, H. Core-shell composites LiCl@SiO<sub>2</sub> for thermochemical energy storage with high storage density, International Renewable Energy Storage Conference (IRES 2020), May 2020, Dusseldorf, Germany.
7. **Shkatulov, A.I.**, Huinink, H., Stabilization of K<sub>2</sub>CO<sub>3</sub> for thermochemical energy storage, 5th International Workshop on Heat-Mass Transfer Advances for energy conservation and pollution control, 13-16 August 2019, Novosibirsk, Russia.
8. **Shkatulov, A.I.**, Houben, J., Huinink, H. Stabilization of K<sub>2</sub>CO<sub>3</sub> in expanded vermiculite for thermochemical energy storage, Eurotherm №112: Advances in Thermal Energy Storage, 15-17 May 2019, Lleida, Spain
9. **Shkatulov, A.I.**, Kim, S.T., Kato, Y., Aristov, Y.I. Adapting the MgO-CO<sub>2</sub> working pair for thermochemical energy storage by doping with salts, Heat Powered Cycles Conference (HPC 2018), 16-19 September 2018, Bayreuth, Germany
10. **Shkatulov, A.I.**, Kardash, T. Aristov, Y.I., Layered double hydroxide Mg-Al-OH for thermochemical heat storage, International Sorption Heat Pump Conference (ISHPC 2017), 7-10 August 2017, Tokyo, Japan
11. **Shkatulov, A.I.**, Aristov, Y.I., Role of surface energy in dehydration of magnesium and calcium hydroxides, XXI International Conference on Chemical Thermodynamics in Russia (RCCT-2017), 26-30 June, Novosibirsk, Russia

12. **Shkatulov, A.I.**, Aristov, Y.I., Thermochemical heat storage by magnesium and calcium hydroxides doped by inorganic salts, Materials Science and Engineering congress (MSE 2016), 27-29 September 2016, Darmstadt, Germany
13. **Shkatulov, A.I.**, Aristov, Y.I., Layered hydroxides as promising candidates for storage of middle-temperature heat, International Symposium on Innovative Materials and Processes for Energy Systems (IMPRES 2016), 4-6 September 2016, Taormina, Italy.
14. **Shkatulov, A.I.**, Aristov, Y.I. Effect of salt additives on decomposition of magnesium and calcium hydroxides, Hot topics of solid-state chemistry (HTSSC-15), 26-28 October 2015, Novosibirsk, Russia.
15. **Shkatulov, A.I.**, Aristov, Y.I., Thermochemical storage of middle temperature heat by magnesium and calcium hydroxides doped by salts: a chemical approach, Sorption Friends, 14-16 September 2015, Milazzo, Italy
16. **Shkatulov, A.I.**, Aristov, Y.I., Salt-doped  $Mg(OH)_2$  and  $Ca(OH)_2$  as candidates for middle-temperature heat storage, Eurotherm №99: Advances in Thermal Energy Storage, 28-30 May 2014, Lleida, Spain
17. **Shkatulov, A.I.**, Aristov, Y.I. Salt-modified calcium hydroxide: a new candidate for middle-temperature heat storage, International Symposium on Innovative Materials and Processes for Energy Systems (IMPRES 2013), 4-6 September 2013, Fukuoka, Japan.
18. **Shkatulov, A.I.**, Ryu, J., Kato, Y., Aristov, Y. New composite “ $Mg(OH)_2$ -vermiculite”: a promising candidate for storage of middle-temperature heat, Heat Powered Cycles, 10-12 September 2012, Alkmaar, the Netherlands