Maltsev Alexey Last update: 2022, September

Birth date: June 30, 1998

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Research interests:

- Density Functional Theory and quantum chemical calculations
- Electronic structures, structure prediction and bond analysis
- Mechanisms of catalytic hydrogen sorption reactions, hydrogen energy and hydrogen
- storage materials
- Rechargeable li-ions and lithium batteries, anode materials and electrolytes
- Rechargeable metal-ions and metal-anode batteries, anode materials and electrolytes

Skills:

- DFT and MD calculations using MOPAC, Gaussian, VASP, Abinit, FHI-Aims, LAMMPS, MLIP programs
- Natural bond analysis using AdNDP2 or multiwfn software
- Kinetic calculations using Transition State Theory, RRKM theory or molecular dynamics
- Fundamental and applied electrochemical energy sources and photovoltaic materials
- Basic python, C, C++

Education:

Oct 2021 – to date	**Skolkovo Institute of Science and Technology** Materials Science and Engineering PhD Program Supervisor: prof. Artem R. Oganov
Sep 2015 – June 2021	**Lomonosov Moscow State University** with Honours Department: Fundamental Physical and Chemical Engineering Major: "Fundamental and Applied Chemistry" Specialization: "New Energy Technologies" GPA 4.8/5

Professional experience:

Jan 2018 – Oct 2021	**Engineer** Chernogolovka, Moscow region, Russia Russian Academy of Sciences, Institute of Problems of Chemical Physics, Department of Functional Materials for Chemical Energy Sources Laboratory of Materials for Hydrogen Energy Storage Competence Center for Technologies of New and Mobile Energy Sources at IPCP RAS

Projects:

2022 – 2024	**Russian Science Foundation (RSCF) project no. 22-73-00219** Компьютерный дизайн новых электролитов для твердотельных аккумуляторов (Computational design of new electrolytes for solid-state batteries)

2018 – 2020	**Russian Foundation for Basic Research project no.18-03-01156** Investigation of the features of the interaction with hydrogen of nanostructured alloys and composites of magnesium with aluminum

Conferences:

2021	XXXIII Scientific Papers Competition for the Prize named after Baturin S.M. **(3rd place)**
2020	**"Lomonosov" Universiade** in Physical and Chemical Engineering // Theoretical modeling of elementary reactions of hydrogenation $Mg_{17}L + H_2$ (L = 3d-metals) (oral presentation) International scientific conference of students and young scientists **"Lomonosov-2020"** // Theoretical modeling of reactions of dissociative addition of hydrogen to magnesium clusters doped with atoms of 3d-transition metals $Mg_{17}L + H_2$ (L = 3d metals) (theses)
2019	Conference "**Physical chemistry in Russia and beyond: from quantum chemistry to experiment**", Chernogolovka, Moscow Region // Theoretical modeling of the reactions of stepwise addition of H_2 molecules to magnesium clusters Mg_{18}, $Ni@Mg_{17}$, $Mg_{17}Ni$ (theses and oral presentation) All-Russian School-Conference for Young Scientists "**Organic and Hybrid Nanomaterials**", Ivanovo State University // Theoretical modeling of elementary reactions of hydrogen interaction with magnesium clusters doped with Ni (theses) **"Lomonosov" Universiade** in Physical and Chemical Engineering // Theoretical modeling of elementary hydrogenation reactions $Mg_{17}Ni + nH_2$ (n = 1-3) (oral presentation) International scientific conference of students and young scientists **"Lomonosov-2019"** // Theoretical modeling of reactions of sequential dissociative addition of hydrogen to a Ni-doped magnesium cluster $Mg_{17}Ni + nH_2$ (n = 1-3) (theses and poster presentation)
2018	"**Physical and chemical problems of renewable energy (RE2018)**", Chernogolovka, Moscow Region, 2018 // Theoretical modeling of dissociative addition of a hydrogen molecule to nickel-doped magnesium $Mg_{17}Ni$ clusters (theses and oral presentation)

Publications:

1. Maltsev A.P., Charkin O.P. // Theoretical Modeling of Stepwise Addition of H2 Molecules to Magnesium Clusters Mg18 and Mg17Ni // Russ. J. Inorg. Chem., 2020, 65, 185–192 https://doi.org/10.1134/S0036023620020114
2. Maltsev A.P., Charkin O.P. // Theoretical Modeling of Addition of H2 Molecules to Magnesium Clusters Mg17L doped with 3*d*-transition metals // Russ. J. Inorg. Chem., 2020 V.65, N.8, P. 1204–1212 https://doi.org/10.1134/S0036023620080100
3. O.P. Charkin, A.P. Maltsev // Density Functional Theory Modeling of Reactions of Addition of H 2 Molecules to Magnesium Clusters Mg 17 M Doped with Atoms M of Transition 3d Elements// J. Phys. Chem. A, 2021, 125, 2308–2315 https://doi.org/10.1021/acs.jpca.1c00211
4. A.P. Maltsev, O.P. Charkin // Theoretical Modeling of Exo- and Endohedral Hydrogenation Reactions of the Doped Magnesium Cluster Mg17Ni // Russ. J. Inorg. Chem., 2021, 66, 12, 1860–1876 https://doi.org/10.1134/S0036023621120111