Curriculum Vitae

Professor Artem R. Oganov, FRSC, MAE

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Personal Information

Address: Skolkovo Institute of Science and Technology, Bolshoy Boulevard 30, bld. 1, 121205 Moscow, Russia.

Email: a.oganov@skoltech.ru

Date of Birth: March 3, 1975

Family Status: Married, four children (daughters Jeanne and Adriana, sons Lev and Alexander).

Languages: Native Russian, fluent English, intermediate French, basic Italian and German.

Professional Experience

2026-Present: Chief Scientific Officer, SberUniversity, Russia

2024–Present: Distinguished Professor, Skolkovo Institute of Science and Technology, Russia.

2015–2024: Professor, Skolkovo Institute of Science and Technology, Russia.

2021–2024: Head of Laboratory of Crystal Chemistry, Institute of Geochemistry and Analytical Chemistry, Russian Academy of Sciences, Moscow, Russia.

2020–2024: Professor, MISIS University, Moscow, Russia (Head of Department of Semiconductors and Dielectrics, 2021–2024).

2017–2020: Founder and Director, International Center for Materials Discovery, Northwestern Polytechnical University, China.

2013–2020: Head of Laboratory and Professor, Moscow Institute of Physics and Technology, Russia.

2008–2017: Professor (2010–2017) and Associate Professor (2008–2010), Department of Geosciences & Institute for Advanced Computational Sciences, Stony Brook University, USA.

2007: Habilitation, Department of Materials, ETH Zurich, Switzerland (recognized as Doctor of Physical & Mathematical Sciences, Russian highest degree, 2016).

2003–2008: Senior Scientist (2003–2007) and Privatdozent (2007–2008), Department of Materials, ETH Zurich, Switzerland.

2002–2003: Research Fellow, University College London, UK.

Education

2002: Ph.D. in Crystallography, University College London, UK.

1997: M.Sc. in Crystallography (magna cum laude), Moscow State University, Russia.

Research Output

Publications: 388 papers, including 5 in *Nature* and 2 in *Science*, and multiple book chapters.

Citations:

- Google Scholar: 46,070 total citations, h-index = 103.
- Researchgate: 40,925 total citations, h-index = 96.
- Web of Science: 33,198 total citations, h-index = 88.

Books: 2 edited volumes on computational materials discovery, 1 collective monograph on history of the Earth, 1 popular science book on chemistry (bestseller).

Invited Lectures: 585 talks, including 96 plenary and keynote lectures at international conferences.

Major Distinctions and Awards

2026:

- Certificate of honor from Russian President

2025:

- “National expert” prize for popularization of science.
- “Russia – land of opportunities” award (in category “Science and Technology”)
- Highly Cited Researcher Award (Clarivate Analytics).
- Inducted to the Academic Council of the International Core Academy of Sciences and Humanities.
- Voice: Main Faces Award (representative of the VYZOV Prize).

2024:

- Highly Cited Researcher Award (Clarivate Analytics).
- Elected Distinguished Professor, Skolkovo Institute of Science and Technology.
- Tianshan Award for Foreign Experts (Xinjiang Province, China).
- Distinguished Scientist of the President's International Fellow Initiative (PIFI), Chinese Academy of Sciences.
- Fellow, International Core Academy of Sciences and Humanities.
- Znanie Award (for science popularization and contributions to education).

2023: National Award for Popularization of Science ("For the Commitment to Science").

2022: Highly Cited Researcher Award (Clarivate Analytics).

2020: Fellow of the American Physical Society and the Royal Society of Chemistry (FRSC).

2019–Present: Ranked annually among the top 2% most cited scientists (Elsevier).

2019: Friendship Award of the Chinese Government.

2017: George Gamow Award, Concord Award, and Member of Academia Europaea (MAE).

2016: Russian Highly Cited Researcher Award (Chemistry, Clarivate Analytics).

2015: Japan Society for the Promotion of Science Invitation Fellow.

2013: Fellow of the Mineralogical Society of America.

2007: Research Excellence Medal, European Mineralogical Union.

2004: European High-Pressure Research Group Award.

2003: Young Scientist Award, European Union of Geosciences.

2002: President's Award, Geological Society of London.

Professional Services

Editorial Roles:

- Executive Editor (Chemistry), *The Innovation* (IF > 25) (2024-).
- Editorial Board Member: *AIMat (2026-), Crystal Science (2026-), AI Agent (2025-), Matter and Radiation and Extremes (2023-).*
- Former membership in editorial boards: *Geochemistry International* (2021-2026), *Crystals* (2020-2024), *Scientific Reports* (2006-2024), *Journal of Superhard Materials* (2009-2022), Associate Editor of *American Mineralogist* (2006-2010).

Advisory Roles:

- Associated member, Computational Physics commission, International Union of Pure and Applied Physics (2024-).
- Member, Science and Technology Council, Rusnano Corporation (2021–).
- Member, academic council of Fersman Mineralogical Museum (Russian Academy of Sciences) (2016-).
- Chairman, Scientific Council of the National Prize for Future Technologies "VYZOV" (2023–2026).
- Co-chairman of the jury, Sustainable Development Young Scientist Award (2024).
- Commission on Crystallography of Materials, IUCr: consultant (2017–2023), founder and chairman (2011-2017).
- Member of Russian President's Council for Science and Education (2017-2020).

Conference Organization: Organized 23 international workshops on crystal structure prediction in France, China, India, Canada, USA, Switzerland, Italy, Iran, Russia. Organized and chaired tens of symposia. Co-chairman of two panels at World Economic Forum (Dalian, June 2017).

Notable Contributions

- Breakthrough in crystal structure prediction: **USPEX** evolutionary algorithm, widely used in materials science, chemistry, physics, geosciences.
- Discovered **novel high-pressure phases** of elements and compounds, including allotropes of many elements, exotic compounds, and record high-temperature superconductors.

- Discovery and prediction of novel **Earth- and planet-forming materials**: $MgSiO_3$ post-perovskite, novel oxide, carbonate, silicate phases, C-H-N-O system under pressure.
- Prediction of likely **molecules** via a combination of evolutionary global optimization and the development of the concept of magic molecules.
- Prediction of novel **superhard, thermoelectric, thermobarrier, non-linear optical**, and other types of materials.
- Refinement of thermochemical and spectroscopic **electronegativity scales**. Extension of the concept of electronegativity to high pressure, and determination of electronegativities and chemical hardnesses of all elements under pressure, to explain anomalies of high-pressure chemistry.

Media and Outreach

- Featured in documentaries: *Watching the Thought Fly* (directed by V. Gerchikov, 2017), *New Element in the Russian Table* (directed by E. Tukhareli, 2019)
- Biographical documentaries about Artem R. Oganov: *Color of the Crystal* (directed by V. Gerchikov, 2012), *Made by Russians* (directed by L. Parfenov, 2015), *House of Scientists: Artem Oganov* (directed by N. Popova, 2018), *Cool Story: Return of the Professor* (directed by T. Mitkova, 2018), *Children of XX century: Artem Oganov* (directed by A. Cherkasov, 2022).
- Ranked among the most influential Russian scie*ntists by Russian Newsweek (2008), Forbes Russia (2011)*, *Russian Reporter (2014)*. Listed as one of the most influential Russians by *GQ (2019)*.

Professors trained

- Yanming Ma (was my postdoc in 2006-2008, now Academician of Chinese Academy of Sciences and President of Zhejiang University, China).
- Qiang Zhu (PhD student in 2009-2013, now Associate Prof. at Univ. Carolina, USA).
- Maribel Nunez Valdez (2015-2016, now Prof. at Frankfurt U., Germany).
- Andriy O. Lyakhov (postdoc in 2007-2011, then Res. Asst. Prof. at Stony Brook U., USA).
- Yu Xie (PhD student in 2007-2010, now Professor at Jilin U., China).
- Fei Qi (postdoc in 2013-2015, now Assoc. Prof. at Xidian U., China).
- Qinggao Wang (postdoc in 2013-2016, now Professor at Henan U., China).
- Xiaohu Yu (postdoc in 2013-2015, now Assoc. Prof. at Henan Normal U., China).
- Huafeng Dong (postdoc in 2013-2015, now Assoc. Prof., Guangdong U. of Tech., China).
- Xiang-Feng Zhou (postdoc in 2012-2015, now Prof. at Yanshan U., China).
- Dongxu Li (visiting scientist in 2013-2014, now Assoc. Prof., Huaqiao U., China).
- Qianku Hu (visiting scientist in 2013-2014, now Asst. Prof. at Henan Polytechnic U., China).
- Xiao Dong (visiting PhD student in 2012-2014, now Prof. at Nankai U., China).
- Qingfeng Zeng (visiting scientist in 2011-2012, now Assoc. Prof., Northwestern Polytechnical U., China).
- Chaohao Hu (visiting scientist in 2011-2012, now Professor at Guilin U. of Electronic Technology, China).
- Weiwei Zhang (visiting scientist in 2011-2013, now Professor at China Agricultural University).
- Feiwu Zhang (PhD student in 2005-2008, now Professor in Inst. Geochemistry, Chinese Acad. Sci.).
- Haiyang Niu (visiting PhD student in 2014, then postdoc in 2015-2016, now Professor at

Northwestern Polytechnical U., China).
- Alexander Kvashnin (postdoc in 2015-2021, now Professor at Skoltech).
- Congwei Xie (PhD student in 2015-2019, now Professor at Xinjiang Technical Institute of Physics and Chemistry, China).

PhD theses supervised: Alexey Maltsev (2022-2026), Majid Zeraati (2021-2025), Dmitrii Semenok (2018-2022), Tao Fan (2018-2022), Zahed Allahyari (2016-2020), Christian Tantardini (2018-2020), Valery Roizen (2015-2019), Congwei Xie (2015-2019), Oleg Feya (2014-2019), Ivan Kruglov (2014-2018), Jin Zhang (2014-2017), Mahdi Davari (2013-2017), Shengnan Wang (2013-2016), Guangrui Qian (2011-2015), Qiang Zhu (2009-2013), Yu Xie (2007-2010), Feiwu Zhang (2005-2008), Colin W. Glass (2006-2009), Donat Adams (2004-2007), Kai H. Hassdenteufel (2003-2006), Daniel Y. Jung (2004-2008).

Doctor of Science theses supervised: Alexander Kvashnin (2021).

Profiles in scientific databases:

ORCID: https://orcid.org/0000-0001-7082-9728

Google Scholar: https://scholar.google.com/citations?user=PqAlzTcAAAAJ&hl=en

Web of Science: https://www.webofscience.com/wos/author/record/O-8234-2019

Researchgate: https://www.researchgate.net/profile/Artem-Oganov

Scopus: https://www.scopus.com/authid/detail.uri?authorId=6701334785

SciProfiles: https://sciprofiles.com/profile/2219577

Colab.ws: https://colab.ws/researchers/R-35BD7-0CB5B-OQ30X

List of Publications by Artem R. Oganov

BOOKS

1. **Oganov, A.R.** (Editor). *Modern Methods of Crystal Structure Prediction*. Berlin: Wiley-VCH, 2010. ISBN: 978-3-527-40939-6.
2. **Oganov, A.R., Saleh, G., Kvashnin, A.G.** (Editors). *Computational Materials Discovery*. Royal Society of Chemistry, 2018. ISBN: 978-1-78262-961-0.
3. **Kuzmin, M.I., Yarmolyuk, V.V., Gladkochub, D.P., Goryachev, N.A., Derevyanko, A.P., Didenko, A.N., Donskaya, T.V., Kravchinsky, V.A., Oganov, A.R., Pisarevsky, S.A.** *Geological Evolution of the Earth: From Space Dust to the Home of Mankind*. Academic Publishing House "Geo", Novosibirsk, 2021. ISSN: 2686-9993. Reprinted by IKI Publishing House, 2026, ISBN 978-5-4344-1103-5 (In Russian).
4. **Oganov, A.R.** *Chemistry*. AST Publishing House, Moscow, 2022. (Popular science book, in Russian). ISBN: 978-5-17-145181-3.

REVIEWS AND CHAPTERS IN BOOKS

1. **Oganov, A.R., Brodholt, J.P., Price, G.D.** *Ab initio theory of thermoelasticity and phase transitions in minerals*. EMU Notes in Mineralogy, Vol. 4 ('Energy Modelling in Minerals', edited by C.M. Gramaccioli), pp. 83–170, 2002.

2. **Oganov, A.R.** *Theory of Minerals at High and Ultrahigh Pressures: Structure, Properties, Dynamics, and Phase Transitions*. In: *High-Pressure Crystallography*, NATO Science Series: II: Mathematics, Physics and Chemistry, Vol. 140, pp. 199–215 (edited by A. Katrusiak, P.F. McMillan). Kluwer Academic Publishers, Dordrecht, 2003.

3. **Oganov, A.R.** *Phase diagrams of minerals from first principles*. Proceedings of the CECAM Workshop «First-Principles Simulations: Perspectives and Challenges in Mineral Sciences» (Berichte aus Arbeitskreisen der DGK, Nr. 14, German Crystallographic Society), pp. 53–62, 2004.

4. **Adams, D.J., Oganov, A.R.** *Theory of minerals at extreme conditions: predictability of structures and properties*. EMU Notes in Mineralogy, Vol. 7 ('High-Pressure Behaviour of Minerals', edited by R. Miletich), pp. 441–457, 2005.

5. **Jung, D.Y., Oganov, A.R.** *Basics of first-principles simulation of matter under extreme conditions*. EMU Notes in Mineralogy, Vol. 7 ('High-Pressure Behaviour of Minerals', edited by R. Miletich), pp. 117–138, 2005.

6. **Oganov, A.R.** *Thermodynamics, phase transitions, equations of state and elasticity of minerals at high pressures and temperatures*. Treatise on Geophysics, Vol. 2 (Mineral Physics, edited by G.D. Price), pp. 121–152, 2007.

7. **Oganov, A.R., Ma, Y., Glass, C.W., Valle, M.** *Evolutionary crystal structure prediction: overview of the USPEX method and some of its applications*. Psi-k Newsletter, No. 84, Highlight of the Month, pp. 142–171, 2007. (Invited review).

8. **Oganov, A.R., Ma, Y., Lyakhov, A.O., Valle, M., Gatti, C.** *Evolutionary crystal structure prediction and novel high-pressure phases*. In: *High-Pressure Crystallography* (eds. E. Boldyreva, P. Dera), pp. 293–325. Springer Verlag, 2010.

9. **Oganov, A.R.** *Crystal structure prediction, a formidable problem*. In: *Modern Methods of Crystal Structure Prediction* (ed. A.R. Oganov), pp. xi–xxi. Berlin: Wiley-VCH, 2010.

10. **Lyakhov, A.O., Oganov, A.R., Valle, M.** *Crystal structure prediction using evolutionary approach*. In: *Modern Methods of Crystal Structure Prediction* (ed. A.R. Oganov), pp. 147–180. Berlin: Wiley-VCH, 2010.

11. **Oganov, A.R., Schön, J.C., Jansen, M., Woodley, S.M., Tipton, W.W., Hennig, R.G.** *First blind test of inorganic crystal structure prediction*. In: *Modern Methods of Crystal Structure Prediction* (ed. A.R. Oganov), pp. 223–231. Berlin: Wiley-VCH, 2010.

12. **Oganov, A.R.** *Boron under pressure: phase diagram and novel high-pressure phase*. In: *Boron Rich Solids*, Chapter 14 (pp. 207–215). Eds. N. Orlovskaya and M. Lugovy. Springer Verlag, Berlin, 2011.

13. **Oganov, A.R.** *Discovery of γ-B_{28}, a Novel Boron Allotrope with Partially Ionic Bonding*. In: *Boron and Boron Compounds – From Fundamentals to Applications*. Materials Research Society, ISBN 978-1-61839-514-6, Chapter 1, pp. 1–15, 2011.

14. **Oganov, A.R., Lyakhov, A.O., Zhu, Q.** *Theory of superhard materials*. In: *Comprehensive Hard Materials Review*, Elsevier, Vol. 3, pp. 59–79, 2014.

15. **Yu, X.H., Oganov, A.R., Wang, Z.H., Saleh, G., Baturin, V.S., Sharma, V., Zhu, Q., Wang, Q.G., Zhou, X.F., Popov, I.A., Boldyrev, A.I.** *Predicting the structure and chemistry of low-dimensional materials*. In: *Handbook of Solid State Chemistry*, Vol. 5, eds. R. Dronskowski, S. Kikkawa, A. Stein, pp. 527–570, 2017.

16. **Dong, X., Oganov, A.R.** *Electrides and their high-pressure chemistry*. In: *Correlations in Condensed Matter Under Extreme Conditions*, ed. G.N.N. Angilella & A. La Magna, Springer Verlag, pp. 69–84, 2017.

17. **Oganov, A.R., Kruglov, I.A., Zhang, J., Davari Esfahani, M.** *Computational materials discovery using evolutionary algorithms*. In: *Computational Materials Discovery*. Eds.: A.R. Oganov, A.G. Kvashnin, G. Saleh. Royal Society of Chemistry, pp. 15–65, 2018.

18. **Oganov, A.R., Kvashnin, A.G., Saleh, G.** *Computational materials discovery: dream or reality?* In: *Computational Materials Discovery*. Eds.: A.R. Oganov, A.G. Kvashnin, G. Saleh. Royal Society of Chemistry, pp. 1–14, 2018.

19. **Allahyari, Z., Oganov, A.R.** *Multi-objective optimization as a tool for materials design*. In: *Handbook of Materials Modeling* (ed. W. Andreoni, S. Yip). Volume 2 Applications: Current and Emerging Materials. Springer Verlag, pp. 2777–2790, 2018.

20. **Kruglov, I.A., Dolgirev, P.E., Oganov, A.R., Mazitov, A.B., Pozdnyakov, S.N., Mazhnik, E.A., Yanilkin, A.V.** *Machine learning interatomic potentials for global optimization and molecular dynamics simulation*. In: *Materials Informatics* (edited by O. Isayev, A. Tropsha, S. Curtarolo), pp. 253–288. Wiley-VCH, 2019.

21. **Oganov, A.R., Konson, G.R.** *The way the people of art and science study the world*. In: *Art History in the Context of Other Sciences in Modern World: Parallels and Interactions* (Proceedings of the international academic conference, April 21–26, 2019), pp. 278–291, 2020.

PAPERS IN REFEREED JOURNALS

368. Kotelevskaya E.Y., Volkova E.A., Shkurskii B.B., Poletaev D.O., Oganov A.R., Krivchuk V.O. Capture of lanthanum atoms by the (111) twin boundary in fluorite: a DFT study. Submitted (2026).

367. Barma D.D., Obrubov A.S., Tudi A., Yang Z., Rybkovskiy D.V., Mikhailova A.A., Oganov A.R. Computational prediction of promising deep-UV nonlinear optical borate fluorides $BaBO_2F$ and $SrBO_2F$. Submitted (2026).

366. Min. J., Li H., Wu X., Lv Y., Li X., Guo J., Oganov A.R., Jia D. Stabilizing active cobalt sites by interstitial carbon and nitrogen co-doping in metallic cobalt for efficient alkaline oxygen evolution reaction. *J. Energy Chem.* **119**, 53-63.

365. Oganov A.R. Atomic electronegativities from electrostatic potentials. *Front. Phys.* **21**, 114200 (2026).

364. Oganov A.R. Pauling's Second Rule and Its Applications: From Inorganic Compounds to Understanding the Function of ATP. *Rep. Natl. Acad. Sci. Rep. Armenia* **126**, 1-7 (2026).

363. Ren C., Ding H., Oganov A.R., Wang Z., Cui H., Song H., Dong X. Predicting twin grain boundaries in molecular crystals using evolutionary algorithm: Application to aspirin, RDX, and HMX. *Phys. Rev.* **B113**, 134110 (2026).

362. Orang A.A., Alaei M., Oganov A.R. Predicting the Curie temperature of magnetic materials with machine learning: Descriptor engineering, graph neural networks, and the role of curated data. *Comp. Mater. Sci.* **269**, 114663 (2026).

361. Oganov A.R. Surprises from a boron-rich semiconductor under pressure. *Nat. Sci. Rev.,* nwag137 (2026).

360. Fedyaeva M., Lepeshkin S., Oganov A.R. Systematic Study of Boron–Nitrogen Molecules: Structures, Stability, and Potential as High-Energy-Density Materials. *J. Clust. Sci.* **37**, 34 (2026).

359. Solodovnikov S.F., Zeraati M., Kuznetsov A.B., Zolotova E.S., Nasyrbaev A.R. Gulyaev I.P., Igumenov I.K., Shutilov R.A., Maksimovsky E.A., Pishchur D.P., Yudin V.N., Lukashov V.V., Korolkov I.V., Maltsev A.P., Oganov A.R. Thermal and mechanical properties of double perovskite-type Ba_2YNbO_6 ceramic. *Ceramics International*, in press (2026).

358. Cheng M., Zhang W., Jin W., Oganov A.R., Yang Z., Pan S. Hydroxyl-induced structural reconstruction: two new potassium hepta-borates with deep-UV transparency and enhanced birefringence. *Inorg. Chem. Frontiers* **13**, 1006-1012. (2026).

357. Dallakyan O.L., Maltsev A.P., Chepkasov I.V., Aghamalyan M.A., Hunanyan A.A., Petrosyan N.Z., Chobanyan M.S., Sahakyan M.T., Khachatryan L.G., Oganov A.R., Zakaryan H.A. Computational screening for novel solid-state electrolytes in Li_3MX_6 composition. *J. Energy Chem.* **112**, 495-504 (2026).

356. Bahrami F., Salimi A., Momenzadeh Abardeh Z., Oganov A.R. Prediction of the crystal structure of avalidomide using machine learning potentials and crystal engineering. *CrystEngComm*. 28, 697-705 (2026).

355. Oganov A.R., Kostenko M.G. Simple electronegativity-based model for predicting formation of stable compounds across the periodic table. *Nature Communications* 17, 929 (2026).

354. Dyachenko A.A., Lukoyanov A.V., Anisimov V.I., Oganov A.R. The impact of electronic correlations on the structural stability and spectral properties of ferrocene and polyferrocene under pressure. *Phys. Chem. Chem. Phys.* **27**, 19703-19709 (2025).

353. Alaei M., Mosleh Z., Rezaei N., Oganov A.R. Experimental exchange interaction dataset for magnetic materials: spin waves to MC simulations. *Sci. Data* **12**, 1832 (2025).

352. Shorikov A.O., Korotin D.M., Anisimov V.I., Oganov A.R. Does covalency decrease with coordination number? *J. Chem. Phys.* **163**, 114106 (2025).

351. Mikhailova A.A., Maltsev A.P., Mendes P.C.D., Zamudio F.B., Oganov A.R., Kozlov S.M. Structure and adsorption properties of Cu-Au nanoparticles in harsh reactive environments. *J. Chem. Phys.* **163,** 124302 (2025).

350. ***Zhao L., Zong H., Oganov A.R., Ding X., Sun J., Ackland G.J.*** Fast crystallization driven by quasiatomic electrons at ultralow temperatures. *Phys. Rev. Lett.* **135**, 116101 (2025).

349*. Mazitov A., Kruglov I., Yanilkin A.V., Arsenin A.V., Volkov V.S., Kvashnin D.G., Oganov A.R., Novoselov K.S.* Substrate-aware computational design of two-dimensional materials. *npj Comp. Mater.* **11**, 270 (2025).

348*. Trukhan E., Mazhnik E., Oganov A.R.* Acceleration of crystal structure relaxation with deep reinforcement learning. *npj Comp. Mater.* **11**, 290 (2025).

347*. Chepkasov I.V., Radina A.D., Baidyshev V.S., Polovinkin M., Rybin N., Shapeev A., Krikorov A.A., Oganov A.R., Dashevsky Z., Kvashnin D.G., Kvashnin A.G.* Tuning of mechanical properties of doped PbTe-based thermoelectric materials driven by intrinsic defect. *J. Mater. Chem.* ***A*****13**, 31170-31180 (2025).

346*. Momenzadeh Abardeh Z., Salimi A., Oganov A.R.* Synthon modularity in crystal structure prediction: designing pomalidomide polymorphs and co-crystals. *CrystEngComm. **27,*** 5514-5526 (2025).

345*. Novoselov D., Korotin D., Mazannikova M., Anisimov V.I., Oganov A.R.* *Towards understanding the* driving forces of the formation of multicomponent compounds: the case of complex oxides. *J. Chem. Phys.* **162**, 204106 (2025).

344. Fedyaeva M., Lepeshkin S., Oganov A.R. First-principles prediction of the structure and stability of boron-carbon clusters. *Comput. Mater. Sci.* **257**, 113952 (2025).

343. Alaei M., Oganov A.R. Optimizing supercell structures for Heisenberg exchange interaction calculations. *Phys. Rev. B* **111**, 144419 (2025).

342. Anisimova E.D., Vaneeva E.E., Baturin V.S., Lepeshkin S.V., Oganov A.R. Structural motifs and evolution of boron nanoclusters. *J. Clust. Sci.* **36**, 98 (2025).

341. Maltsev A.P., Iosimovska A.V., Chepkasov I.V., Oganov A.R. Structure transformations and ionic conductivity in germanides of sodium and potassium. *J. Mater. Chem. A* **13**, 14612-14619 (2025).

340. Rezaei N., Alaei M., Oganov A.R. Evaluating SCAN and r^2SCAN meta-GGA functionals for predicting transition temperatures in antiferromagnetic materials. *Phys. Rev. B* **111**, 144406 (2025).

339. Alaei M., Sobieszczyk P., Ptok A., Rezaei N., Oganov A.R., Qaiumzadeh A. Origin of A-type antiferromagnetism and chiral split magnons in altermagnetic α-MnTe. *Phys. Rev. B* **111**, 104416 (2025).

338. Zeraati M., Oganov A.R., Maltsev A.P., Solodovnikov S.F. Computational screening of complex oxides for next-generation thermal barrier coatings. *J. Appl. Phys.* **137**, 065106 (2025).

337. Vaneeva E.E., Lepeshkin S.V., Rybkovskiy D.V., Oganov A.R. Exploring the diversity of molecular carbon oxides, and their potential as energy density materials. *Mater. Today Energy* **46**, 101821 (2025).

336. Alkabakibi Y., Barma D.D., Rybkovskiy D.V., Tudi A., Xie C., Oganov A.R. Computational identification of four promising nonlinear optical materials for near and middle ultraviolet operation. *JETP Lett.* **121**, 256–261 (2025).

335. Chang L., Tamaki H., Yokoyama T., Wakasugi K., Yotsuhashi S., Kusaba M., Oganov A.R., Yoshida R. Shotgun crystal structure prediction using machine-learned formation energies. *npj Comput. Mater.* **10**, 298 (2024).

334. Fan T., Oganov A.R. Combining machine-learning models with first-principles high-throughput calculations to accelerate the search for promising thermoelectric materials. *J. Mater. Chem. C* **13**, 1439–1448 (2025).

333. Hou J., Cui H., Oganov A.R., Li H., Weng X., Zhou X.-F., Wang H.-T., Dong X. H_4O^{2+} ion stabilized by pressure. *Phys. Rev. B* **109**, 174102 (2024).

332. Momenzadeh Abardeh Z., Bahrami F., Oganov A.R. Predicting co-crystal structures of N-halide phthalimides with 3,5-dimethylpyridine. *Acta Crystallogr. B* **80**, 620–627 (2024).

331. Hunniset L.M., ..., Oganov A.R., ... The seventh blind test of crystal structure prediction: structure ranking methods. *Acta Crystallogr. B* **80**, 548–574 (2024).

330. Hunniset L.M., ..., Oganov A.R., ... The seventh blind test of crystal structure prediction: structure generation methods. *Acta Crystallogr. B* **80**, 517–547 (2024).

329. Kong J., Shi K., Oganov A.R., Zhang J., Su L., Dong X. Exotic compounds of monovalent calcium synthesized at high pressure. *Matter Radiat. Extremes* **9**, 067803 (2024).

328. Fedyaeva M., Lepeshkin S.V., Chukanov N.V., Oganov A.R. Mutual transformations of polysulfide chromophore species in sodalite-group minerals: a DFT study of S_6 decomposition. *ChemPhysChem*, e202400532 (2024).

327. Jalolov F.N., Podryabinkin E.V., Oganov A.R., Shapeev A.V., Kvashnin A.G. Mechanical properties of single and polycrystalline solids from machine learning. *Adv. Theory Simul.* **7**, 2301171 (2024).

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