

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

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

Citations:

- Google Scholar: 43,892 total citations, h-index = 100.
- Web of Science: 31,662 total citations, h-index = 86.

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: 573 talks, including 92 plenary and keynote lectures at international conferences.

Major Distinctions and Awards

2025:

- “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).
- Editorial Board Member: *AI Agent, Matter at Radiation and Extremes, Geochemistry International*.
- Former membership in editorial boards: *Crystals* (2020-2024), *Scientific Reports* (2006-2024), *Journal of Superhard Materials* (2009-2022), Associate Editor of *American Mineralogist* (2006-2010).

Advisory Roles:

- Chairman, Scientific Council of the National Prize for Future Technologies "VYZOV" (2023–Present).
- Co-chairman of the jury, Sustainable Development Young Scientist Award (2024).
- Member, Science and Technology Council, Rusnano Corporation (2021–Present).
- Member, academic council of Fersman Mineralogical Museum (Russian Academy of Sciences) (2016-).
- Member of the Commission on Science Popularization at Russian Academy of Sciences (2025-).
- Associated member, Computational Physics commission, International Union of Pure and Applied Physics (2024-2026).
- 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 scientists 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: Majid Zeraati (2021-2025), Dmitrii Semenov (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=PgAlzTcAAAAJ&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. (In Russian).
 4. **Oganov, A.R.** *Chemistry*. AST Publishing House, Moscow, 2022. (Popular science book, in Russian). ISBN: 978-5-17-145181-3.
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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 -B₂₈, 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.
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PAPERS IN REFEREED JOURNALS

- 361. 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).
- 360. 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).
- 359. 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*, <https://doi.org/10.1039/D5QI02044A> (2025).
- 358. 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. Submitted. (2025).
- 357. 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. In prep. (2025).
- 356. Barma D.D., Obruchov 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 (2025).
- 355. Bahrami F., Salimi A., Momenzadeh Abardeh Z., Oganov A.R.** Prediction of the crystal structure of avadomide using machine learning potentials and crystal engineering. *CrystEngComm.*, in press. (2025).
- 354. Oganov A.R., Kostenko M.G.** Simple electronegativity-based model for predicting formation of stable compounds across the periodic table. *Nature Communications*, in press (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 quasiautomatic 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.* **A13**, 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^2 SCAN 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. Hunnisset L.M., ..., Oganov A.R., ... The seventh blind test of crystal structure prediction: structure ranking methods. *Acta Crystallogr. B* **80**, 548–574 (2024).

330. Hunnisset 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 S₆ 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).

326. Novoselov D.Yu., Korotin D.M., Shorikov A.O., Anisimov V.I., Oganov A.R. Electronic correlations and intrinsic magnetism of interstitial quasi-atomic states in Li₈Au electride. *Phys. Chem. Chem. Phys.* **26**, 17854–17859 (2024).

325. Zhou D., Semenok D., Galasso M., Alabarse F.G., Sannikov D., Troyan I.A., Nakamoto Y., Shimizu K., Oganov A.R. Raisins in a hydrogen pie: ultrastable cesium and rubidium polyhydrides. *Adv. Energy Mater.* **14**, 2400077 (2024).

324. Anisimov V.I., Oganov A.R., Korotin D.M., Novoselov D.Y., Shorikov A.O., Belozerov A.S. First-principles definition of ionicity and covalency in molecules and solids. *J. Chem. Phys.* **160**, 144113 (2024).

323. Rybkovskiy D.V., Lepeshkin S.V., Mikhailova A.A., Baturin V.S., Oganov A.R. Lithiation of phosphorus at the nanoscale: a computational study of Li_nP_m clusters. *Nanoscale* **16**, 1197–1205 (2024).

322. Banaru D.A., Aksenov S.M., Banaru A.M., Oganov A.R. Mutual correlations of complexity indices of the crystal structure for the series of mercury-containing minerals. *Z. Krist.* **239**, 207–215 (2024).

321. Iosimovska A.V., Maltsev A.P., Chepkasov I.V., Oganov A.R. Thermodynamic stability and ionic conductivity in lithium-germanium binary system. *Appl. Phys. Lett.* **124**, 163904 (2024).

320. Zeraati M., Oganov A.R., Fan T., Solodovnikov S.F. Searching for low thermal conductivity materials for thermal barrier coatings: A theoretical approach. *Phys. Rev. Mater.* **8**, 033601 (2024).

319. Chepkasov I.V., Kvashnin A.G., Radina A.D., Matsokin N.A., Jalolov F.N., Oganov A.R., Dashevsky Z. Origin of brittle behavior of doped PbTe-based thermoelectric materials. *Appl. Phys. Lett.* **124**, 022104 (2024).

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