

Curriculum Vitae

Professor Artem R. Oganov, FRSC, MAE

(Updated: December 6, 2025)

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: 43,852 total citations, h-index = 100.
- Web of Science: 31,618 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: 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=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.
-

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.

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).

318. Maltsev A.P., Chepkasov I.V., Oganov A.R. New promising class of anode materials for Ca-ion battery: Polyaromatic hydrocarbons. *Mater. Today Energy* **39**, 101467 (2024).

317. Shutov G.M., Semenok D.V., Kruglov I.A., Oganov A.R. Ternary superconducting hydrides in the La-Mg-H system. *Mater. Today Phys.* **40**, 101300 (2024).

316. Korotin D.M., Novoselov D.Y., Shorikov A.O., Anisimov V.I., Oganov A.R. Electronic correlations in the ultranarrow energy band compound Pb₉Cu(PO₄)₆O: A DFT+DMFT study. *Phys. Rev. B* **108**, L241111 (2023).

315. Hao C.-M., Li X., Oganov A.R., Hou J., Ding S., Ge Y., Wang L., Dong X., Wang H.-T., Yang G., Zhou X.-F., Tian Y. Superconductivity in compounds of sodium-intercalated graphite. *Phys. Rev. B* **108**, 214507 (2023).

314. Novoselov D.Y., Mazannikova M.A., Korotin D.M., Shorikov A.O., Anisimov V.I., Oganov A.R. Exploring correlation effects and volume collapse during electride dimensionality change in Ca₂N. *Phys. Chem. Chem. Phys.* **25**, 30960–30965 (2023).

313. Mazannikova M.A., Korotin D.M., Anisimov V.I., Oganov A.R., Novoselov D.Y. Dimensionality-driven evolution of electronic structure and transport properties in pressure-induced phases of Ca₂N electride. *JETP Lett.* **118**, 651–657 (2023).

312. Kruglov I.A., Yanilkin A.V., Propad Y., Mazitov A.B., Rachitskii P., Oganov A.R. Crystal structure prediction at finite temperatures. *npj Comput. Mater.* **9**, 197 (2023).

311. Vaneeva E.E., Lepeshkin S.V., Oganov A.R. Prediction and rationalization of abundant C-N-H molecules in different environments. *J. Phys. Chem. Lett.* **14**, 8367–8375 (2023).

310. Maltsev A.P., Chepkasov I.V., Oganov A.R. Order-disorder phase transition and ionic conductivity in a Li₂B₁₂H₁₂ solid electrolyte. *ACS Appl. Mater. Interfaces* **15**, 42511–42519 (2023).

309. Mikhailova A.A., Lepeshkin S.V., Baturin V.S., Maltsev A.P., Uspenskii Y.A., Oganov A.R. Ultralow

- reaction barriers for CO oxidation in Cu-Au nanoclusters. *Nanoscale* **15**, 13699–13707 (2023).
- 308. Huang H.-M., Zhu Q., Blatov V.A., Oganov A.R., Wei H., Jiang P., Li Y.-L.** Novel topological motifs and superconductivity in Li-Cs system. *Nano Lett.* **23**, 5012–5018 (2023).
- 307. Chen W., Huang X., Semenok D.V., Chen S., Zhang K., Oganov A.R., Cui T.** Enhancement of the superconducting critical temperature realized in the La-Ce-H system at moderate pressures. *Nat. Commun.* **14**, 2660 (2023).
- 306. Maltsev A.P., Chepkasov I.V., Kvashnin A.G., Oganov A.R.** Ionic conductivity of lithium phosphides. *Crystals* **13**, 756 (2023).
- 305. Pozdnyakov S., Oganov A.R., Mazhnik E., Mazitov A., Kruglov I.** Fast general two- and three-body interatomic potential. *Phys. Rev. B* **107**, 125160 (2023).
- 304. Fedyaeva M., Lepeshkin S., Oganov A.R.** Stability of sulfur molecules and insights into sulfur allotropy. *Phys. Chem. Chem. Phys.* **25**, 9294–9299 (2023).
- 303. Anisimov V.I., Oganov A.R., Mazannikova M.A., Novoselov D.Yu., Korotin D.M.** Formal valence, charge distribution and chemical bond in a compound with a high oxidation state: KMnO_4 . *JETP Lett.* **117**, 377–383 (2023).
- 302. Rachitskii P., Kruglov I., Finkelstein A.V., Oganov A.R.** Protein structure prediction using the evolutionary algorithm USPEX. *Proteins* **91**, 843–853 (2023).
- 301. Zhou D., Semenok D.V., Volkov M.A., Troyan I.A., Seregin A.Yu., Chepkasov I.V., Sannikov D.A., Lagoudakis P.G., Oganov A.R., German K.E.** Synthesis of technetium hydride $\text{TcH}_{1.3}$ at 27 GPa. *Phys. Rev. B* **107**, 064102 (2023).
- 300. Rybkovskiy D.V., Lepeshkin S.V., Baturin V.S., Mikhailova A.A., Oganov A.R.** Phosphorus nanoclusters and insight into the formation of phosphorus allotropes. *Nanoscale* **15**, 1338–1346 (2023).
- 299. Galasso M., Oganov A.R.** Automag: An automatic workflow software for calculating the ground magnetic state of a given structure and estimating its critical temperature. *Comput. Phys. Commun.* **283**, 108571 (2023).
- 298. Hou J., Dong X., Oganov A.R., Weng X.-J., Hao C.-M., Yang G., Wang H.-T., Zhou X.-F., Tian Y.** Helium-bearing superconductor at high pressure. *Phys. Rev. B* **106**, L220501 (2022).
- 297. Xie C.W., Tudi A., Oganov A.R.** PNO: a promising deep-UV nonlinear optical material with the largest second harmonic generation effect. *Chem. Commun.* **58**, 12491–12494 (2022).
- 296. Marchenko E.A., Oganov A.R., Mazhnik E.A., Eremin N.N.** Stable compounds in the $\text{CaO-Al}_2\text{O}_3$ system at high pressures. *Phys. Chem. Miner.* **49**, 44 (2022).
- 295. Troyan I.A., Semenok D.V., Ivanova A.G., Kvashnin A.G., Zhou D., Sadakov A.V., Sobolevsky O.A., Pudalov V.M., Lyubutin I.S., Oganov A.R.** High-temperature superconductivity in hydrides. *Phys.-Usp.* **65**, 799–813 (2022).
- 294. Rahmanian Koshkaki S., Allahyari Z., Oganov A.R., Solozhenko V.L., Polovov I., Belozеров A., Katanin A., Anisimov V.I., Tikhonov E., Qian G.R., Maksimtshev K., Mukhamadeev A., Chukin A., Korolev A., Mushnikov N., Li H.** Computational prediction of new magnetic materials. *J. Chem. Phys.* **157**, 124704 (2022).
- 293. Rybin N., Chepkasov I., Novoselov D.Y., Anisimov V.I., Oganov A.R.** Prediction of stable silver fluorides. *J. Phys. Chem. C* **126**, 15057–15063 (2022).
- 292. Momenzadeh-Abardeh Z., Salimi A., Oganov A.R.** Crystal structure prediction of N-halide phthalimide compounds: halogen bonding synthons as a touchstone. *CrystEngComm* **24**, 6066–6075 (2022).
- 291. Semenok D.V., Troyan I.A., Sadakov A.V., Zhou D., Galasso M., Kvashnin A.G., Kruglov I.A., Bykov A.A., Terent'ev K.Y., Cherepanin A.V., Sobolevskiy O.A., Pervakov K.S., Seregin A.Yu., Helm T., Förster T., Grochowiak A.D., Tozer S.W., Nakamoto Y., Shimizu K., Pudalov V.M., Lyubutin I.S., Oganov A.R.** Effect of magnetic impurities on superconductivity in LaH_{10} . *Adv. Mater.* **34**, 2204038 (2022).
- 290. Lepeshkin S.V., Naumova A.S., Baturin V.S., Oganov A.R.** "Magic" molecules and a new look at chemical diversity of hydrocarbons. *J. Phys. Chem. Lett.* **13**, 7600–7606 (2022).
- 289. Semenok D.V., Chen W., Huang X., Zhou D., Kruglov I.A., Mazitov A.B., Galasso M., Tantardini C., Gonze X., Kvashnin A.G., Oganov A.R., Cui T.** Sr-doped molecular hydrogen: synthesis and properties of SrH_{22} . *Adv. Mater.* **34**, 2200924 (2022).
- 288. Novoselov D.Y., Mazannikova M.A., Korotin D.M., Shorikov A.O., Korotin M.A., Anisimov V.I., Oganov A.R.** Localization mechanism of interstitial electronic states in electride mayenite. *J. Phys. Chem.*

Lett. **13**, 7155–7160 (2022).

- 287. Wang Y., Bykov M., Chepkasov I., Samtsevitch A., Bykova E., Zhang X., Jiang S.-q., Greenberg E., Chariton S., Prakapenka V.B., Oganov A.R., Goncharov A.F.** Stabilization of hexazine rings in potassium polynitride at high pressure. *Nat. Chem.* **14**, 794–800 (2022).
- 286. Dong X., Oganov A.R., Cui H., Zhou X.-F., Wang H.-T.** Electronegativity and chemical hardness of the elements under pressure. *Proc. Natl. Acad. Sci.* **119**, e2117416119 (2022).
- 285. Boeri L., Hennig R.G., Hirschfeld P.J., Profeta G., Sanna A., Zurek E., Pickett W.E., Amsler M., Dias R., Eremets M., Heil C., Hemley R.J., Liu H., Ma Y., Pierleoni C., Kolmogorov A., Rybin N., Novoselov D., Anisimov V.I., Oganov A.R., Pickard C.J., Bi T., Arita R., Errea I., Pellegrini C., Requist R., Gross E.K.U., Margine E.R., Xie S.R., Quan Y., Hire A., Fanfarillo L., Stewart G.R., Hamlin J.J., Stanev V., Gonnelli R.S., Piatti E., Romanin D., Daghero D., Valenti R.** The 2021 room-temperature superconductivity roadmap. *J. Phys.: Condens. Matter* **34**, 183002 (2022).
- 284. Li H.F., Oganov A.R., Cui H., Zhou X.-F., Dong X., Wang H.-T.** Ultrahigh-pressure magnesium hydrosilicates as reservoirs of water in early Earth. *Phys. Rev. Lett.* **128**, 035703 (2022).
- 283. Dyachenko A.A., Lukoyanov A.V., Anisimov V.I., Oganov A.R.** Electride properties of ternary silicide and germanide of La and Ce. *Phys. Rev. B* **105**, 085146 (2022).
- 282. Li X., Niu H., Oganov A.R.** COPEX: co-evolutionary crystal structure prediction algorithm for complex systems. *npj Comput. Mater.* **7**, 199 (2021).
- 281. Popov Z.I., Tikhomirova K.A., Demin V.A., Chowdhury S., Oganov A.R., Kvashnin A.G., Kvashnin D.G.** Novel two-dimensional boron oxynitride predicted using USPEX evolutionary algorithm. *Phys. Chem. Chem. Phys.* **23**, 26178–26184 (2021).
- 280. Stavrou E., Maryewski A.A., Lobanov S.S., Oganov A.R., Konopkova Z., Prakapenka V.B., Goncharov A.F.** Ethane and methane at high pressures: structure and stability. *J. Chem. Phys.* **155**, 184503 (2021).
- 279. Zhang J., Li X., Dong X., Dong H., Oganov A.R., McMahon J.M.** Theoretical study of the crystal structure, stability and properties of phases in the V-N system. *Phys. Rev. B* **104**, 134111 (2021).
- 278. Semenok D.V., Troyan I.A., Ivanova A.G., Kvashnin A.G., Hanfland M., Sadakov A.V., Sobolevskiy O.A., Pervakov K.S., Lyubutin I.S., Glazyrin K.V., Giordano N., Karimov D.N., Vasiliev A.L., Akashi R., Pudalov V.M., Oganov A.R.** Superconductivity at 253 K in lanthanum-yttrium ternary hydrides. *Mater. Today* **48**, 18–28 (2021).
- 277. Mazitov A.B., Oganov A.R.** Grain boundaries in minerals: atomic structure, phase transitions, and effect on strength of polycrystals. *Zap. Ross. Mineral. Obs.* **150**, 92–102 (2021).
- 276. Samtsevich A.I., Oganov A.R.** Mechanisms of phase transitions in Al_2SiO_5 phases. *Zap. Ross. Mineral. Obs.* **150**, 79–91 (2021).
- 275. Fan T., Oganov A.R.** Discovery of high performance thermoelectric chalcogenides through first-principles high-throughput screening. *J. Mater. Chem. C* **9**, 13226–13235 (2021).
- 274. Chen W., Semenok D.V., Huang X., Shu H., Li X., Duan D., Cui T., Oganov A.R.** High-Temperature Superconducting Phases in Cerium Superhydride with a T_c up to 115 K below a Pressure of 1 Megabar. *Phys. Rev. Lett.* **127**, 117001 (2021).
- 273. Novoselov D.Y., Korotin D.M., Shorikov A.O., Anisimov V.I., Oganov A.R.** Interacting electrons in two-dimensional electride Ca_2N . *J. Phys. Chem. C* **125**, 15724–15729 (2021).
- 272. Sandu M.P., Kovtunov M.A., Baturin V.S., Kurzina I., Oganov A.R.** Influence of Pd:Bi ratio on Pd-Bi/ Al_2O_3 catalysts: structure, surface and activity in glucose oxidation. *Phys. Chem. Chem. Phys.* **23**, 14889–14897 (2021).
- 271. Rybin N., Novoselov D.Y., Korotin D.M., Anisimov V.I., Oganov A.R.** Novel copper fluoride analogs of cuprates. *Phys. Chem. Chem. Phys.* **23**, 15989–15993 (2021).
- 270. Yue C., Weng X.-J., Gao G., Oganov A.R., Dong X., Shao X., Wang X., Sun J., Xu B., Wang H.-T., Zhou X.-F., Tian Y.** Formation of copper boride on Cu(111). *Fundam. Res.* **1**, 482–487 (2021).
- 269. Korotin D.M., Novoselov D.Y., Anisimov V.I., Oganov A.R.** Mixed spin $S=1$ and $S=1/2$ layered lattice in Cu_2F_5 . *Phys. Rev. B* **104**, 064410 (2021).
- 268. Tantardini C., Oganov A.R.** Thermochemical electronegativities of the elements. *Nat. Commun.* **12**, 2087 (2021).
- 267. Kun L., Wang J., Oganov A.R.** High-pressure phase diagram of the Ti-O system. *J. Phys. Chem. Lett.* **12**, 5486–5493 (2021).

- 266. Novoselov D.Y., Anisimov V.I., Oganov A.R.** Strong electronic correlations in interstitial magnetic centers of zero-dimensional electride $\beta\text{-Yb}_5\text{Sb}_3$. *Phys. Rev. B* **103**, 235126 (2021).
- 265. Naumova A.S., Lepeshkin S.V., Bushlanov P.V., Oganov A.R.** Unusual chemistry of the C-H-N-O system under pressure and implications for giant planets. *J. Phys. Chem. A* **125**, 3936–3942 (2021).
- 264. Fan T., Oganov A.R.** AICON2: A program for calculating transport properties quickly and accurately. *Comput. Phys. Commun.* **266**, 108027 (2021).
- 263. Li K., Wang J., Blatov V.A., Gong Y., Umezawa N., Tada T., Hosono H., Oganov A.R.** Crystal and electronic structure engineering of tin monoxide by external pressure. *J. Adv. Ceram.* **10**, 565–577 (2021).
- 262. Li H., Min J., Yang Z., Wang Z., Pan S., Oganov A.R.** Prediction of Novel van der Waals Boron Oxides with Superior Deep-Ultraviolet Nonlinear Optical Performance. *Angew. Chem. Int. Ed.* **60**, 10791–10797 (2021).
- 261. Troyan I.A., Semenok D.V., Kvashnin A.G., Sadakov A.V., Sobolevskiy O.A., Pudalov V.M., Ivanova A.G., Prakapenka V.B., Greenberg E., Gavrilyuk A.G., Lyubutin I.S., Struzhkin V.V., Bergara A., Errea I., Bianco R., Calandra M., Mauri F., Monacelli L., Akashi R., Oganov A.R.** Anomalous high-temperature superconductivity in YH_6 . *Adv. Mater.* **33**, 2006832 (2021).
- 260. Knyazev A., Savushkin I., Mirsaidov U., Lukoyanov A., Oganov A.** Synthesis and structure of triple thorium phosphates with monazite structure. *J. Radioanal. Nucl. Chem.* **327**, 1105–1112 (2021).
- 259. Hou J., Weng X.J., Oganov A.R., Shao X., Gao G., Dong X., Wang H.T., Zhou X.F., Tian Y.** Helium-Induced Nitrogen Salt at High Pressure. *Phys. Rev. B* **103**, L060102 (2021).
- 258. Chen W., Semenok D.V., Kvashnin A.G., Huang X., Kruglov I.A., Galasso M., Song H., Duan D., Goncharov A.F., Prakapenka V.B., Oganov A.R., Cui T.** Synthesis of Molecular Metallic Barium Superhydride: Pseudocubic BaH_{12} . *Nat. Commun.* **12**, 273 (2021).
- 257. Semenok D.V., Zhou D., Kvashnin A.G., Huang X., Galasso M., Kruglov I.A., Ivanova A.G., Gavriliuk A.G., Chen W., Tkachenko N.V., Boldyrev A.I., Troyan I., Oganov A.R., Cui T.** Novel Strongly Correlated Europium Superhydrides. *J. Phys. Chem. Lett.* **12**, 32–40 (2021).
- 256. Wang Y., Glazyrin K., Roizen V., Oganov A.R., Chernyshov I., Zhang X., Greenberg E., Prakapenka V.B., Yang X., Jiang S.-q., Goncharov A.F.** Novel Hydrogen Clathrate Hydrate. *Phys. Rev. Lett.* **125**, 255702 (2020).
- 255. Allahyari Z., Oganov A.R.** Nonempirical definition of Mendeleev numbers: organizing the chemical space. *J. Phys. Chem. C* **124**, 23867–23878 (2020).
- 254. Chen W.H., Semenok D.V., Troyan I.A., Ivanova A.G., Huang X.L., Oganov A.R., Cui T.** Superconductivity and equation of state of lanthanum at megabar pressures. *Phys. Rev. B* **102**, 134510 (2020).
- 253. Zhu S.C., Yan X.Z., Oganov A.R., Zhu Q.** A revisited mechanism of the graphite-to-diamond transition at high temperature. *Matter* **3**, 864–878 (2020).
- 252. Ostanin I.A., Oganov A.R., Magnanimo V.** Collapse modes in simple cubic and body-centered cubic arrangements of elastic beads. *Phys. Rev. E* **102**, 032901 (2020).
- 251. Broadway D.A., Scholten S.C., Tan C., Dontschuk N., Lillie S.E., Johnson B.C., Zheng G., Wang Z., Oganov A.R., Tian S., Li C., Lei H., Wang L., Hollenberg L.C.L., Tetienne J.-P.** Imaging domain reversal in an ultrathin van der Waals ferromagnet. *Adv. Mater.* **32**, 2003314 (2020).
- 250. Kvashnin A.G., Tantardini C., Zakaryan H.A., Kvashnina Yu.A., Oganov A.R.** Computational search for new W-Mo-B compounds. *Chem. Mater.* **32**, 7028–7035 (2020).
- 249. Miao N., Wang J., Gong Y., Wu J., Niu H., Wang S., Li K., Oganov A.R., Tada T., Hosono H.** Computational prediction of boron-based MAX phases and MXene derivatives. *Chem. Mater.* **32**, 6947–6957 (2020).
- 248. Novoselov D., Korotin D., Shorikov A.O., Oganov A.R., Anisimov V.I.** Weak Coulomb correlations stabilize the electride high-pressure phase of elemental calcium. *J. Phys.: Condens. Matter* **32**, 445501 (2020).
- 247. Mazhnik E., Oganov A.R.** Application of machine learning methods for predicting new superhard materials. *J. Appl. Phys.* **128**, 075102 (2020).
- 246. Pakhnova M.S., Kruglov I., Yanilkin A., Oganov A.R.** Search for stable cocrystals of energetic materials using the evolutionary algorithm USPEX. *Phys. Chem. Chem. Phys.* **22**, 16822–16830 (2020).
- 245. Kvashnin A.G., Rybkovskiy D.V., Filonenko V.P., Bugakov V.I., Zibrov I.P., Brazhkin V.V., Oganov A.R.,**

- Osiptsov A.A., Zakirov A.Ya.** WB_{5-x} : synthesis, properties, and crystal structure - new insights into the long-debated compound. *Adv. Sci.* **7**, 2000775 (2020).
- 244. Cherednichenko K.A., Mukhanov V.A., Wang Z., Oganov A.R., Kalinko A., Dovgaliuk I., Solozhenko V.L.** Discovery of new boron-rich chalcogenides: orthorhombic B_6X ($X=S, Se$). *Sci. Rep.* **10**, 9277 (2020).
- 243. Tikhomirova K.A., Tantardini C., Sukhanova E.V., Popov Z.I., Evlashin S.A., Tarkhov M.A., Zhdanov V.L., Dudin A.A., Oganov A.R., Kvashnin D.G., Kvashnin A.G.** Exotic two-dimensional structure: the first case of hexagonal NaCl. *J. Phys. Chem. Lett.* **11**, 3821–3827 (2020).
- 242. Shorikov A., Skorniyakov S.L., Anisimov V.I., Oganov A.R.** Electronic correlations in uranium hydride UH_5 under pressure. *J. Phys.: Condens. Matter* **32**, 385602 (2020).
- 241. Allahyari Z., Oganov A.R.** Coevolutionary search for optimal materials in the space of all possible compounds. *npj Comput. Mater.* **5**, 55 (2020).
- 240. Fan T., Oganov A.R.** AICON: a program for calculating thermal conductivity quickly and accurately. *Comput. Phys. Commun.* **251**, 107074 (2020).
- 239. Zhang J., McMahon J.M., Oganov A.R., Li X.F., Dong X., Dong H.F., Wang S.N.** High-temperature superconductivity in the Ti-H system at high pressures. *Phys. Rev. B* **101**, 134108 (2020).
- 238. Semenok D.V., Kruglov I.A., Savkin I.A., Kvashnin A.G., Oganov A.R.** On distributions of superconductivity in metal hydrides. *Curr. Opin. Solid State Mater. Sci.* **24**, 100808 (2020).
- 237. Salke N.P., Davari Esfahani M.M., Yedukondalu N., Zhang Y., Kruglov I.A., Zhou J., Greenberg E., Prakapenka V.B., Liu J., Oganov A.R., Lin J.F.** Prediction and synthesis of dysprosium hydride phases at high pressure. *Inorg. Chem.* **59**, 5303–5312 (2020).
- 236. Rybkovskiy D.V., Kvashnin A.G., Kvashnina Yu.A., Oganov A.R.** Structure, stability, and mechanical properties of boron-rich Mo-B phases: a computational study. *J. Phys. Chem. Lett.* **11**, 2393–2401 (2020).
- 235. Zhou D., Semenok D.V., Duan D., Xie H., Chen W., Huang X., Li X., Liu B., Oganov A.R., Cui T.** Superconducting praseodymium superhydrides. *Sci. Adv.* **6**, eaax6849 (2020).
- 234. Zhou D., Semenok D.V., Xie H., Huang X., Duan D., Aperis A., Oppeneer P.M., Galasso M., Kartsev A.I., Kvashnin A.G., Oganov A.R., Cui T.** High-pressure synthesis of magnetic neodymium superhydrides. *J. Am. Chem. Soc.* **142**, 2803–2811 (2020).
- 233. Semenok D.V., Kvashnin A.G., Ivanova A.G., Svitlyk V., Fominski V.Yu., Sadakov A.V., Sobolevskiy O.A., Pudalov V.M., Troyan I.A., Oganov A.R.** Superconductivity at 161 K in thorium hydride ThH_{10} : synthesis and properties. *Mater. Today* **33**, 36–44 (2020).
- 232. Kruglov I.A., Semenok D.V., Song H., Szczesniak R., Wrona I.A., Akashi R., Davari Esfahani M.M., Duan D., Cui T., Kvashnin A.G., Oganov A.R.** Superconductivity of LaH_{10} and LaH_{16} polyhydrides. *Phys. Rev. B* **101**, 024508 (2020).
- 231. Semenok D., Oganov A.R.** Measuring Meissner effect at megabar pressures. *Natl. Sci. Rev.* **6**, 856 (2019).
- 230. Kruglov I.A., Yanilkin A., Oganov A.R., Korotaev P.** Phase diagram of uranium from ab initio calculations and machine learning. *Phys. Rev. B* **100**, 174104 (2019).
- 229. Kvashnin A.G., Kvashnin D.G., Oganov A.R.** Novel unexpected reconstructions of (100) and (111) surfaces of NaCl: theoretical prediction. *Sci. Rep.* **9**, 14267 (2019).
- 228. Mazhnik E., Oganov A.R.** Models of hardness and fracture toughness of solids. *J. Appl. Phys.* **126**, 125109 (2019).
- 227. Salke N., Davari Esfahani M.M., Zhang Y., Kruglov I.A., Zhou J., Wang Y., Greenberg E., Prakapenka V.B., Liu J., Oganov A.R., Lin J.-F.** Synthesis of clathrate cerium superhydride CeH_9 below 100 GPa with atomic hydrogen sublattice. *Nat. Commun.* **10**, 4453 (2019).
- 226. Naumova A.S., Lepeshkin S.V., Oganov A.R.** Hydrocarbons under pressure: phase diagrams and surprising new compounds in the C-H system. *J. Phys. Chem. C* **123**, 20497–20501 (2019).
- 225. Kvashnin A.G., Allahyari Z., Oganov A.R.** Computational discovery of hard and superhard materials. *J. Appl. Phys.* **126**, 040901 (2019).
- 224. Novoselov D.Y., Korotin D.M., Shorikov A.O., Oganov A.R., Anisimov V.I.** Interplay between the Coulomb interaction and hybridization in Ca and anomalous pressure dependence of the resistivity. *JETP Lett.* **109**, 387–391 (2019).
- 223. Xie C.W., Zhang Q., Zakaryan H.A., Wan H., Liu N., Kvashnin A.G., Oganov A.R.** Stable and hard hafnium borides: A first-principles study. *J. Appl. Phys.* **125**, 205109 (2019).

- 222. Oganov A.R., Pickard C.J., Zhu Q., Needs R.J.** Structure prediction drives materials discovery. *Nat. Rev. Mater.* **4**, 331–348 (2019).
- 221. Niu H.Y., Niu S.W., Oganov A.R.** Simple and accurate model of fracture toughness of solids. *J. Appl. Phys.* **125**, 065105 (2019).
- 220. Zhu M.H., Weng X.J., Gao G., Dong S., Ling L.F., Wang W.H., Zhu Q., Oganov A.R., Dong X., Tian Y.J., Zhou X.F., Wang H.T.** Magnetic borophenes from an evolutionary search. *Phys. Rev. B* **99**, 205412 (2019).
- 219. Podryabinkin E.V., Tikhonov E.V., Shapeev A.V., Oganov A.R.** Accelerating crystal structure prediction by machine-learning interatomic potentials with active learning. *Phys. Rev. B* **99**, 064114 (2019).
- 218. Lepeshkin S.V., Baturin V.S., Uspenskii Yu.A., Oganov A.R.** Method for simultaneous prediction of atomic structure of nanoclusters in a wide area of compositions. *J. Phys. Chem. Lett.* **10**, 102–106 (2019).
- 217. Dong B.J., Wang Z.H., Hung N.T., Oganov A.R., Yang T., Saito R., Zhang Z.D.** New two-dimensional phase of tin chalcogenides: Candidates for high-performance thermoelectric materials. *Phys. Rev. Mater.* **3**, 013405 (2019).
- 216. Bushlanov P.V., Blatov V.A., Oganov A.R.** Topology-based crystal structure generator. *Comput. Phys. Commun.* **236**, 1–7 (2019).
- 215. Oganov A.R.** Crystal structure prediction: reflections on present status and challenges. *Faraday Discuss.* **211**, 643–660 (2018).
- 214. Kvashnin A.G., Semenok D.V., Kruglov I.A., Wrona I.A., Oganov A.R.** High-temperature superconductivity in a Th-H system under pressure conditions. *ACS Appl. Mater. Interfaces* **10**, 43809–43816 (2018).
- 213. Yu X.H., Oganov A.R., Zhu Q., Qian G.R.** The stability and unexpected chemistry of oxide clusters. *Phys. Chem. Chem. Phys.* **20**, 30437–30444 (2018). (Corrigendum: *Phys. Chem. Chem. Phys.* **21**, 1623).
- 212. Dong H.F., Oganov A.R., Brazhkin V.V., Wang Q.G., Zhang J., Davari Esfahani M.M., Zhou X.F., Wu F.G., Zhu Q.** Boron oxides under pressure: Prediction of the hardest oxides. *Phys. Rev. B* **98**, 174109 (2018).
- 211. Zhao C.M., Duan Y.F., Gao J., Liu W.J., Dong H.M., Dong H.F., Zhang D.K., Oganov A.R.** Unexpected stable phases of tungsten borides. *Phys. Chem. Chem. Phys.* **20**, 24665–24670 (2018).
- 210. Kruglov I.A., Kvashnin A.G., Goncharov A.F., Oganov A.R., Lobanov S.S., Holtgrewe N., Jiang S.Q., Prakapenka V.B., Greenberg E., Yanilkin A.V.** Uranium polyhydrides at moderate pressures: prediction, synthesis, and expected superconductivity. *Sci. Adv.* **4**, eaat9776 (2018).
- 209. Shorikov A.O., Roizen V.V., Oganov A.R., Anisimov V.I.** Role of temperature and Coulomb correlation in the stabilization of CsCl-type phase in FeS under pressure. *Phys. Rev. B* **98**, 094112 (2018).
- 208. Streltsov S.V., Roizen V.V., Ushakov A.V., Oganov A.R., Khomskii D.I.** Old puzzle of incommensurate crystal structure of calaverite AuTe₂ and predicted stability of novel AuTe compound. *Proc. Natl. Acad. Sci. USA* **115**, 9945–9950 (2018).
- 207. Feya O.D., Wang Q.G., Lepeshkin S.V., Baturin V.S., Uspenskii Yu.A., Oganov A.R.** Tetrahedral honeycomb surface reconstructions of quartz, cristobalite and stishovite. *Sci. Rep.* **8**, 11947 (2018).
- 206. Oganov A.R.** 2D materials worth their salt. *Nat. Chem.* **10**, 694–695 (2018).
- 205. Yao X., Xie C.W., Dong D., Oganov A.R., Zeng Q.F.** Novel high-pressure calcium carbonates. *Phys. Rev. B* **98**, 014108 (2018).
- 204. Kvashnin A.G., Zakaryan H., Zhao C.M., Duan Y.F., Kvashnina Y.A., Xie C.W., Dong H.F., Oganov A.R.** New tungsten borides, their stability and outstanding mechanical properties. *J. Phys. Chem. Lett.* **9**, 3470–3477 (2018).
- 203. Mazitov A., Oganov A.R., Yanilkin A.V.** Titanium-hydrogen interaction at megabar pressure. *J. Appl. Phys.* **123**, 235901 (2018).
- 202. Frolov T., Setyawan W., Kurtz R., Marian J., Oganov A.R., Rudd R.E., Zhu Q.** Grain boundary phases in bcc metals. *Nanoscale* **10**, 8253–8268 (2018).
- 201. Fan T., Xie C.W., Wang S.Y., Oganov A.R., Cheng L.F.** First-principles study of thermoelectric properties of Mg₂Si-Mg₂Pb semiconductor materials. *RSC Adv.* **8**, 17168–17175 (2018).
- 200. Cherednichenko K.A., Kruglov I.A., Oganov A.R., Le Godec Y., Mezouar M., Solozhenko V.L.** Boron monosulfide: equation of state and pressure-induced phase transition. *J. Appl. Phys.* **123**, 135903 (2018).

199. Semenok D.V., Kvashnin A.G., Kruglov I.A., Oganov A.R. Actinium hydrides AcH_{10} , AcH_{12} , AcH_{16} as high-temperature conventional superconductors. *J. Phys. Chem. Lett.* **9**, 1920–1926 (2018).
198. He X.L., Dong X., Wu Q.S., Zhao Z.S., Zhu Q., Oganov A.R., Tian Y.J., Yu D.L., Zhou X.F., Wang H.T. Predicting the ground-state structure of sodium boride. *Phys. Rev. B* **97**, 100102 (Rapid Communications) (2018).
197. He X.L., Weng H.J., Zhang Y., Zhao Z.S., Wang Z.H., Xu B., Oganov A.R., Tian Y.J., Zhou X.F., Wang H.T. Two-dimensional boron on Pb (110) surface. *FlatChem* **7**, 34–41 (2018).
196. Hu X.B., Niu H.Y., Ma X.L., Oganov A.R., Fisher C.A.J., Sheng N.C., Liu J.D., Jin T., Sun X.F., Ikuhara Y. Atomic-scale observation and analysis of chemical ordering in M_3B_2 and M_5B_3 borides. *Acta Materialia* **149**, 274–284 (2018).
195. Kvashnin A.G., Kruglov I.A., Semenok D.V., Oganov A.R. Iron superhydrides FeH_5 and FeH_6 : stability, electronic properties and superconductivity. *J. Phys. Chem. C* **122**, 4731–4736 (2018).
194. James A., Davari Esfahani M.M., Woerner W.R., Sinclair A., Ehm L., Oganov A.R., Parise J.B. Theoretical and experimental investigations into novel oxynitride discovery in the GaN-TiO₂ system at high pressure. *Crystals* **8**, 15 (2018).
193. Walsh D.W., Butler K.T., Skelton J.M., Xie C.W., Oganov A.R., Walsh A. Computer-aided design of metal chalcogenide semiconductors: from chemical composition to crystal structure using data-mining and evolutionary global optimisation. *Chem. Science* **9**, 1022–1030 (2018).
192. Nunez-Valdez M., Allahyari Z., Oganov A.R. Efficient technique for computational design of thermoelectric materials. *Comp. Phys. Comm.* **222**, 152–157 (2018).
191. Kruglov I., Akashi R., Yoshikawa S., Oganov A.R., Davari M. Refined phase diagram of the H-S system with high-T_c superconductivity. *Phys. Rev. B* **96**, 220101 (Rapid Comm.) (2017).
190. Khrapov N., Roizen V., Posypkin M., Samtsevich A., Oganov A.R. Volunteer computing for computational materials design. *Lobachevskii J. Mathem.* **38**, 926–930 (2017).
189. Kruglov I., Sergeev O., Yanilkin A., Oganov A.R. Energy-free machine learning force field for aluminum. *Sci. Rep.* **7**, 8512 (2017).
188. Lobanov S.S., Dong X., Martirosyan N.S., Samtsevich A.I., Stevanovic V., Gavryushkin P.V., Litasov K.D., Greenberg E., Prakapenka V.B., Oganov A.R., Goncharov A.F. Raman spectroscopy and X-ray diffraction of sp^3 -CaCO₃ at lower mantle pressures. *Phys. Rev. B* **96**, 104101 (2017).
187. Zakaryan H.A., Kvashnin A.G., Oganov A.R. Stable reconstruction of the (110) surface and its role in pseudocapacitance of rutile-like RuO₂. *Sci. Rep.* **7**, 10357 (2017).
186. Gou H.Y., Zhu L., Huang H.T., Biswas A., Keefer D.W., Chaloux B.L., Prescher C., Yang L.X., Kim D.Y., Ward M.D., Lerach J., Wang S.N., Oganov A.R., Epshteyn A., Badding J.V., Strobel T.A. From Linear Molecular Chains to Extended Polycyclic Networks: Polymerization of Dicyanoacetylene. *Chem. Mater.* **29**, 6706–6718 (2017).
185. Yu S.Y., Huang B., Zeng Q.F., Oganov A.R., Zhang L.T., Frapper G. Emergence of novel polynitrogen molecule-like species, covalent chains and layers in magnesium-nitrogen Mg_xN_y phases under high pressure. *Phys. Chem. Chem. Phys.* **121**, 11037–11046 (2017).
184. Shtukenberg A.G., Zhu Q., Carter D.J., Vogt L., Hoja J., Schneider E., Song H.X., Pokroy B., Polishchuk I., Tkatchenko A., Oganov A.R., Rohl A.L., Tuckerman M.E., Kahr B. Powder diffraction and crystal structure prediction identify four new coumarin polymorphs. *Chemical Science* **8**, 4926–4940 (2017).
183. Li B.X., Qian G.R., Oganov A.R., Boulfelfel S.E., Faller R. Mechanism of the fcc-hcp phase transformation in solid Ar. *J. Chem. Phys.* **146**, 214502 (2017).
182. Bazhanova Z.G., Roizen V.V., Oganov A.R. High-pressure behavior of the Fe-S system and composition of the Earth's inner core. *Physics-Uspekhi* **60**, 1025–1032 (2017).
181. Esfahani Davari M.M., Zhu Q., Dong H.F., Oganov A.R., Wang S.N., Rakitin M.S., Zhou X.F. Novel magnesium borides and their superconductivity. *Phys. Chem. Chem. Phys.* **19**, 14486–14494 (2017).
180. Zeng Q.F., Yu S.Y., Li D., Oganov A.R., Frapper G. Emergence of novel hydrogen chlorides under high pressure. *Phys. Chem. Chem. Phys.* **19**, 8236–8242 (2017).
179. Esfahani Davari M.M., Niu H.Y., Zhang J., Oganov A.R. Decomposition of solid germane under high pressure and unexpected chemistry of germanium hydrides with superconductivity. *Phys. Rev. B* **95**, 134506 (2017).
178. Zhang J., Oganov A.R., Li X.F., Dong H.F., Davari Esfahani M.M. First-principles investigation of Zr-O

compounds, their crystal structures and mechanical properties. *J. Appl. Phys.* **121**, 155104 (2017).

177. Wang D.H., Zhou H.Y., Hu C.H., Zhong Y., Oganov A.R., Rao G.H. Prediction of thermodynamically stable Li-B compounds at ambient pressure. *Phys. Chem. Chem. Phys.* **19**, 8471–8477 (2017).

176. Yu S.Y., Zeng Q.F., Niu H.Y., Huang B., Oganov A.R., Frapper G., Zhang L.T. First-principles study of Zr-N crystalline phases: phase stability, electronic and mechanical properties. *RSC Advances* **7**, 4697–4703 (2017).

175. Kvashnin A.G., Oganov A.R., Allahyari Z. Computational search for novel hard chromium-based materials. *J. Phys. Chem. Lett.* **8**, 755–764 (2017).

174. Zhang J., Oganov A.R., Li X.F., Niu H.Y. Novel pressure-stabilized hafnium nitrides, and their properties. *Phys. Rev. B* **95**, 020103(R) (Rapid Communications) (2017).

173. Dong X., Oganov A.R., Goncharov A.F., Stavrou E., Lobanov S., Saleh G., Qian G.R., Zhu Q., Gatti C., Deringer V., Dronskowski R., Zhou X.-F., Prakapenka V., Konopkova Z., Popov I., Boldyrev A.I., Wang H.T. A stable compound of helium and sodium at high pressure. *Nature Chemistry* **9**, 440–445 (2017).

172. Stavrou E., Lobanov S.V., Dong H.F., Oganov A.R., Prakapenka V.B., Konopkova Z., Goncharov A.F. Synthesis of ultra-incompressible sp^3 -hybridized carbon nitride with 1:1 stoichiometry. *Chem. Mater.* **28**, 6925–6033 (2016).

171. Lepeshkin S., Baturin V., Tikhonov E., Matsko N., Uspenskii Y., Naumova A., Feyta O., Schoonen M.A., Oganov A.R. Super-oxidation of silicon nanoclusters: magnetism and reactive oxygen species at the surface. *Nanoscale* **8**, 1816–1820 (2016).

170. Zhu J., Oganov A.R., Feng W.X., Yao Y.G., Zhang S.J., Yu X.H., Zhu J.L., Yu R.C., Jin C.Q., Dai X., Fang Z., Zhao Y.S. Pressure-induced Ag_2Te polymorphs in conjunction with topological non-trivial to metal transition. *AIP Advances* **6**, 085003 (2016).

169. Saleh G., Oganov A.R. Pressure-induced stabilization of carbonic acid and other compounds in the C-H-O phase diagram. *Sci. Rep.* **6**, 32486 (2016).

168. Dong H.F., Oganov A.R., Wang Q.G., Wang S.N., Wang Z.H., Zhang J., Davari Esfahani M.M., Zhou X.F., Wu F.G., Zhu Q. Prediction of a new ground state of superhard compound B_6O at ambient conditions. *Sci. Rep.* **6**, 31288 (2016).

167. Matsko N.L., Tikhonov E.V., Baturin V.S., Lepeshkin S.V., Oganov A.R. The impact of electron correlations on the energetics and stability of silicon nanoclusters. *J. Chem. Phys.* **145**, 074313 (2016).

166. Dolgirev P.E., Kruglov I.A., Oganov A.R. Machine learning scheme for fast extraction of interatomic potentials and chemistry. *AIP Advances* **6**, 085318 (2016).

165. An Q., Reddy K.M., Dong H.F., Chen M.-W., Oganov A.R., Goddard, W.A. III. Nanotwinned boron suboxide (B_6O): new ground state of B_6O . *Nano Letters* **16**, 4236–4242 (2016).

164. Goncharov A.F., Lobanov S.S., Kruglov I.A., Zhao X.M., Chen X.J., Oganov A.R., Konopkova Z., Prakapenka V.B. Hydrogen sulfide at high pressure: change in stoichiometry. *Phys. Rev. B* **93**, 174105 (2016).

163. Qian G.R., Niu H.Y., Hu C.H., Oganov A.R., Zeng Q.F., Zhou H.Y. Prediction of unique diversity of stable hydronitrogens, and implication for planetary and materials sciences. *Sci. Rep.* **6**, 25947 (2016).

162. Reilly A.M., Cooper R.I., ..., Oganov A.R., ... Groom C.R. Report on the sixth blind test of organic crystal structure prediction methods. *Acta Cryst B* **72**, 439–459 (2016).

161. Yu S.Y., Huang B., Jia X.J., Oganov A.R., Zeng Q.F., Zhang L.T., Frapper G. Exploring the real ground-state structures of molybdenum-nitrogen MoN_2 phases. *J. Phys. Chem. C* **120**, 11060–11067 (2016).

160. Zhang W.W., Oganov A.R., Zhu Q., Lobanov S., Stavrou E., Goncharov A.F. Stability of numerous novel potassium chlorides at high pressure. *Sci. Rep.* **6**, 26265 (2016).

159. Wang Q.G., Oganov A.R., Zhu Q., Feyta O.D., Ma D.W. Unexpectedly rich structures of rutile $TiO_2(011)-(2\times 1)$ and driving forces behind their formations: an ab initio evolutionary study. *Phys. Chem. Chem. Phys.* **18**, 19549–19556 (2016).

158. Xie C.W., Oganov A.R., Dong D., Zeng Q.F. A first-principles study of the structural and mechanical properties of stable zirconium carbides. *Phys. Chem. Chem. Phys.* **18**, 12299–12306 (2016).

157. Zhu Q., Shtukenberg A., Carter D., Yu T.Q., Yang J.X., Chen M., Raiteri P., Oganov A.R., Pokroy B., Polishchuk I., Bygrave P., Day G., Rohl A., Tuckerman M., Kahr B. Resorcinol Crystallization from the Melt: A New Ambient Phase and New “Riddles”. *J. Am. Chem. Soc.* **138**, 4881–4889 (2016).

156. Woerner B.R., Qian G.R., Oganov A.R., Stephens P.W., Dharmagunawardhane H.A.N., Sinclair A., Parise J.B. Combined theoretical and in situ scattering strategies for optimized discovery and recovery of

high-pressure phases: a case study of the GaN-Nb₂O₅ system. *Inorg. Chem.* **55**, 3384–3392 (2016).

155. Davari Esfahani M.M., Wang Z.H., Oganov A.R., Dong H.F., Zhu Q., Wang S.N., Rakitin M.S., Zhou X.F. Superconductivity of novel tin hydrides (Sn_nH_m) under pressure. *Sci. Rep.* **6**, 22873 (2016).

154. Wang Q.G., German K.E., Oganov A.R., Dong H.F., Feya O.D., Zubavichus Y.V., Murzin V. Explaining stability of transition metal carbides – and why TcC does not exist. *RSC Advances* **6**, 16197–16202 (2016).

153. Zhou X.F., Oganov A.R., Wang Z.H., Popov I.A., Boldyrev A.I., Wang H.T. Two-dimensional magnetic boron. *Phys. Rev. B* **93**, 085406 (2016).

152. Wang S.N., Oganov A.R., Qian G.R., Zhu Q., Dong H.F., Davari Esfahani M.M. Novel superhard B-C-O phases predicted from first principles. *Phys. Chem. Chem. Phys.* **18**, 1859–1863 (2016).

151. Saleh G., Oganov A.R. Alkali subhalides: High-pressure stability and interplay between metallic and ionic bonds. *Phys. Chem. Chem. Phys.* **18**, 2840–2849 (2016).

150. Yu X.H., Oganov A.R., Popov I.A., Qian G.R., Boldyrev I.A. Antiferromagnetic stabilization in Ti₈O₁₂ cluster. *Angew. Chem. Int. Ed.* **55**, 1699–1703 (2016).

149. Zhu Q., Oganov A.R., Zeng Q.F., Zhou X.F. Structure prediction and its applications in computational materials design. *Chem. Model.* **12**, 219–248 (2016).

148. Mannix A.J., Zhou X.F., Kiraly B., Wood J.D., Alducin D., Myers B., Liu X.L., Fisher B.L., Santiago U., Guest J.R., Yacaman M.J., Ponce-Pedraza A., Oganov A.R., Hersam M.C., Guisinger N.P. Synthesis of borophene: An anisotropic, two-dimensional boron allotrope. *Science* **350**, 1513–1516 (2015).

147. Niu H.Y., Oganov A.R., Chen X.Q., Li D.Z. Novel stable compounds in the Mg-Si-O system under exoplanet pressures and their implications in planetary science. *Sci. Rep.* **5**, 18347 (2015).

146. Xie C.W., Oganov A.R., Dong D., Li D., Debela T.T., Liu N., Zeng Q.F. Rational design of inorganic dielectric materials with expected permittivity. *Sci. Rep.* **5**, 16769 (2015).

145. Yu S.Y., Zeng Q.F., Frapper G., Oganov A.R., Zhang L.T. Pressure-driven formation and stabilization of the superconductive chromium hydrides. *Sci. Rep.* **5**, 17764 (2015).

144. Zhang J., Oganov A.R., Li Z.F., Xue K.H., Wang Z.H., Dong H.F. Prediction of a new ground state of superhard compound B₆O at ambient conditions. *Phys. Rev. B* **92**, 184104 (2015).

143. Li D.X., Oganov A.R., Dong X., Zhou X.F., Zhu Q., Qian G.R., Dong H.F., Li R.K. Nitrogen oxides under pressure: stability, ionization, polymerization, and superconductivity. *Sci. Rep.* **5**, 16311 (2015).

142. Zhu Q., Oganov A.R., Lyakhov A.O., Yu X.X. Generalized evolutionary metadynamics for sampling energy landscapes and its applications. *Phys. Rev. B* **92**, 024106 (2015).

141. Lobanov S.S., Zhu Q., Holtgrewe N., Prescher C., Prakapenka V.B., Oganov A.R., Goncharov A.F. Stable magnesium peroxide at high pressure. *Sci. Rep.* **5**, 13582 (2015).

140. Shen Y.Q., Oganov A.R., Qian G.R., Zhang J., Dong H.F., Zhu Q., Zhou Z.X. Novel lithium-nitrogen compounds at ambient and high pressures. *Sci. Rep.* **5**, 14204 (2015).

139. Rakitin M.S., Oganov A.R., Niu H.Y., Esfahani Davari M.M., Zhou X.F., Qian G.R., Solozhenko V.L. A novel phase of beryllium fluoride at high pressure. *Phys. Chem. Chem. Phys.* **17**, 26283–26288 (2015).

138. Wang Z.H., Zhou X.F., Zhang X.M., Zhu Q., Dong H.F., Zhao M.W., Oganov A.R. Phagraphene: a low-energy graphene allotrope composed of 5-6-7 carbon rings with distorted Dirac cones. *Nano Lett.* **15**, 6182–6186 (2015).

137. Yu X.H., Oganov A.R., Popov I.A., Boldyrev A.I. d-AO spherical aromaticity in Ce₆O₈. *J. Comput. Chem.* **37**, 103–109 (2015).

136. Chen P.C., Wang N., Oganov A.R., Duan W.H. Effects of ferroelectric polarization on surface phase diagram: evolutionary algorithm study of BaTiO₃(001) surface. *Phys. Rev. B* **92**, 085432 (2015).

135. Goncharov A.F., Holtgrewe N., Qian G.R., Hu C.H., Oganov A.R., Somayazulu M., Stavrou E., Pickard C.J., Berlie A., Yen F., Mahmood M., Lobanov S.S., Konopkova Z., Prakapenka V.B. The backbone N_xH compounds at high pressures. *J. Chem. Phys.* **142**, 214308 (2015).

134. Stavrou E., Chen X.J., Oganov A.R., Wang A.F., Yan Y.J., Luo X.G., Chen X.H., Goncharov A.F. Formation of As-As interlayer bonding in the collapsed tetragonal phase of NaFe₂As₂ under pressure. *Sci. Rep.* **5**, 9868 (2015).

133. Zhang J., Oganov A.R., Li X.F., Zeng Q.F., Dong H.F. Novel compounds in the Zr-O system, their crystal structures and mechanical properties. *Phys. Chem. Chem. Phys.* **17**, 17301–17310 (2015).

132. Yu S.Y., Zeng Q.F., Oganov A.R., Frapper G., Zhang L.T. Phase stability, mechanical properties and chemical bonding of titanium nitrides: A first-principles study. *Phys. Chem. Chem. Phys.* **17**, 11763–11769 (2015).

- 131. Dong H.F., Oganov A.R., Zhu Q., Qian G.R.** The phase diagram and hardness of carbon nitrides. *Sci. Rep.* **5**, 9870 (2015).
- 130. Li Y.L., Wang S.N., Oganov A.R., Gou H.Y., Smith J.S., Strobel T.A.** Diverse chemistry of stable calcium carbides. *Nature Communications* **6**, 6974 (2015).
- 129. Zeng Z.D., Zeng Q.F., Liu N., Oganov A.R., Zeng Q.S., Cui Y., Mao W.L.** A new phase of $\text{Li}_{15}\text{Si}_4$ synthesized under pressure. *Adv. Energy Mat.* **5**, 1500214 (2015).
- 128. Liu Y., Wang S.N., Oganov A.R., Zhu Q., Dong X., Kresse G.** Prediction of new thermodynamically stable aluminum oxides. *Sci. Rep.* **5**, 9518 (2015).
- 127. Xu C.S., Xu B., Yang Y.R., Dong H.F., Oganov A.R., Wang S.Y., Duan W.H., Gu B.L., Bellaiche L.** Prediction of a stable post-post-perovskite structure from first principles. *Phys. Rev. B* **91**, 020101 (Rapid Communications) (2015).
- 126. Zhu Q., Oganov A.R., Zeng Q.F.** Formation of stoichiometric CsF_n compounds. *Sci. Rep.* **5**, 7875 (2015).
- 125. Wang Q.G., Oganov A.R., Zhu Q., Zhou X.F.** Novel reconstructions of the (110) surface of rutile TiO_2 predicted by an evolutionary method. *Phys. Rev. Lett.* **113**, 266101 (2014).
- 124. Zhou X.F., Oganov A.R., Shao X., Zhu Q., Wang H.T.** Unexpected reconstruction of the α -boron (111) surface. *Phys. Rev. Lett.* **113**, 176101 (2014).
- 123. Zhu Q., Oganov A.R., Zhou X.F.** Crystal structure prediction and its application in Earth and materials sciences. *Topics in Current Chemistry* **345**, 223–256 (2014).
- 122. Yu S.Y., Zeng Q.F., Oganov A.R., Hu C.H., Frapper G., Zhang L.T.** Exploration of stable compounds, crystal structures, and superconductivity in the Be-H system. *AIP Advances* **4**, 107118 (2014).
- 121. Zhang J., Zeng Q.F., Oganov A.R., Dong D., Y.F. Li** High throughput exploration of $\text{Zr}_x\text{Si}_{1-x}\text{SiO}_4$ dielectrics by evolutionary first-principles approaches. *Phys. Lett. A* **378**, 3549–3554 (2014).
- 120. Zhu Q., Sharma V., Oganov A.R., Ramprasad R.** Predicting polymeric crystal structures by evolutionary algorithms. *J. Chem. Phys.* **141**, 154102 (2014).
- 119. Wang D.H., Zhou H.Y., Hu C.H., Oganov A.R., Zhong Y., Rao G.H.** BaC: a thermodynamically stable layered superconductor. *Phys. Chem. Chem. Phys.* **16**, 20780–20784 (2014).
- 118. Sharma V., Wang C., Zhu Q., Pilania G., Oganov A.R., Ramprasad R.** First-principles design of advanced polymer dielectrics. *Nature Communications* **5**, 4845 (2014).
- 117. Xie C.W., Zeng Q.F., Oganov A.R., Dong D.** Discovering low-permittivity materials: evolutionary search for novel MgAl_2O_4 polymorphs. *Appl. Phys. Lett.* **105**, 022907 (2014).
- 116. Raza Z., Errea I., Oganov A.R., Saitta A.M.** Superconducting metallic skutterudite-type phosphorus nitride at high pressure from first-principles calculations. *Sci. Rep.* **4**, 5889 (2014).
- 115. Qian G.R., Lyakhov A.O., Zhu Q., Oganov A.R., Dong X.** Novel hydrogen hydrate structures under pressure. *Sci. Rep.* **4**, 5606 (2014).
- 114. Strobel T., Kurakevych O., Kim D.Y., Le Godec Y., Crichton W., Guignard G., Guignot N., Cody G., Oganov A.R.** Synthesis of $\beta\text{-Mg}_2\text{C}_3$: a monoclinic high-pressure polymorph of magnesium sesquicarbide. *Inorg. Chem.* **53**, 7020–7027 (2014).
- 113. Zhu Q., Feya O.D., Boulfelfel S.E., Oganov A.R.** Metastable host-guest structure of carbon. *J. Superhard Mater.* **36**, 246–256 (2014).
- 112. Solozhenko V.L., Kurakevych O.O., Kurnosov A., Oganov A.R.** Boron phosphide under pressure: in situ study by Raman scattering and X-ray diffraction. *J. Appl. Phys.* **116**, 033501 (2014).
- 111. Niu H., Chen X.Q., Ren W., Zhu Q., Oganov A.R., Li D., Li Y.** Variable-composition structure prediction and experimental verification of MnB_3 and MnB_4 . *Phys. Chem. Chem. Phys.* **16**, 15866–15873 (2014).
- 110. Xie C.W., Zeng Q.F., Dong D., Gao S., Cai Y., Oganov A.R.** First-principles calculations of the dielectric and vibrational properties of ferroelectric and paraelectric BaAl_2O_4 . *Phys. Lett. A* **378**, 1867–1870 (2014).
- 109. Zhao Z., Wang S., Oganov A.R., Chen P.C., Liu Z., Mao W.L.** Tuning the crystal structure and electronic states of Ag_2Se : structural transitions and metallization under pressure. *Phys. Rev. B* **89**, 180102 (2014).
- 108. Baturin V.S., Lepeshkin S.V., Matsko N.L., Oganov A.R., Uspenskii Yu.A.** Prediction of the atomic structure and stability for the ensemble of silicon nanoclusters passivated by hydrogen. *Europhys. Lett.* **106**, 37002 (2014).

107. Zhou X.F., Dong X., Oganov A.R., Zhu Q., Tian Y.J., Wang H.T. Semimetallic two-dimensional boron allotrope with massless Dirac fermions. *Phys. Rev. Lett.* **112**, 085502 (2014).
106. Xie Y., Li Q., Oganov A.R., Wang H. Superconductivity of lithium-doped hydrogen under high pressure. *Acta Cryst. C* **70**, 104–111 (2014).
105. Zeng Q.F., Oganov A.R., Lyakhov A.O., Xie C.W., Zhang X.D., Zhang J., Zhu Q., Wei B.Q., Grigorenko I., Zhang L.T., Cheng L.F. Evolutionary search for new high-k dielectric materials: methodology and applications to hafnia-based oxides. *Acta Cryst. C* **70**, 76–84 (2014).
104. Finkelstein G.J., Dera P.K., Jahn S., Oganov A.R., Holl C.M., Meng Y., Duffy T.S. Phase transitions and equation of state of forsterite to 90 GPa from single-crystal X-ray diffraction and molecular modeling. *Am. Mineral.* **99**, 35–43 (2014).
103. Zhang W.W., Oganov A.R., Goncharov A.F., Zhu Q., Boulfelfel S.E., Lyakhov A.O., Somayazulu M., Prakapenka V.B., Konopkova Z. Unexpected stoichiometries of stable sodium chlorides. *Science* **342**, 1502–1505 (2013).
102. Zeng Q.F., Peng J.H., Oganov A.R., Zhu Q., Xie C.W., Zhang X.D., Dong D., Zhang L., Cheng L.F. Prediction of stable hafnium carbides: their stoichiometries, mechanical properties and electronic structure. *Phys. Rev. B* **88**, 214107 (2013).
101. Zhu Q., Li L., Oganov A.R., Allen P.B. Evolutionary method for prediction of surface reconstructions with variable stoichiometry. *Phys. Rev. B* **87**, 195317 (2013).
100. Qian G.R., Dong X., Zhou X.-F., Tian Y., Oganov A.R., Wang H.-T. Variable cell nudged elastic band method for studying solid-solid structural phase transitions. *Comp. Phys. Comm.* **183**, 2111–2118 (2013).
99. Zhu Q., Oganov A.R., Lyakhov A.O. Novel stable compounds in the Mg-O system under high pressure. *Phys. Chem. Chem. Phys.* **15**, 7796–7700 (2013).
98. Hu C.H., Oganov A.R., Zhu Q., Qian G.R., Frapper G., Lyakhov A.O., Zhou H.Y. Pressure-induced stabilization and insulator-superconductor transition of BH. *Phys. Rev. Lett.* **110**, 165504 (2013).
97. Hu M., Zhao Z.S., Tian F., Oganov A.R., Wang Q.Q., Xiong M., Fan Q.Z., Wen B., He J.L., Yu D.L., Wang H.-T., Xu B., Tian Y.J. Compressed carbon nanotubes: a family of new multifunctional carbon allotropes. *Sci. Rep.* **3**, 1331 (2013).
96. Oganov A.R., Hemley R.J., Hazen R.M., Jones A.P. Structure, Bonding, and Mineralogy of Carbon at Extreme Conditions. *Rev. Mineral. Geochem.* **75**, 47–77 (2013).
95. Lyakhov A.O., Oganov A.R., Stokes H.T., Zhu Q. New developments in evolutionary structure prediction algorithm USPEX. *Comp. Phys. Comm.* **184**, 1172–1182 (2013).
94. Zhu Q., Jung D.Y., Oganov A.R., Gatti C., Glass C.W., Lyakhov A.O. Stability of xenon oxides at high pressures. *Nature Chemistry* **5**, 61–65 (2013).
93. Zhou X.-F., Oganov A.R., Qian G.R., Zhu Q. First-principles determination of the structure of magnesium borohydride. *Phys. Rev. Lett.* **109**, 245503 (2012).
92. Boulfelfel S.E., Zhu Q., Oganov A.R. Novel sp^3 -forms of carbon predicted by evolutionary metadynamics and analysis of their synthesizability using transition path sampling. *J. Superhard Mater.* **34**, 350–359 (2012).
91. Zhu Q., Zeng Q., Oganov A.R. Systematic search for low-enthalpy sp^3 carbon allotropes using evolutionary metadynamics. *Phys. Rev. B* **85**, 201407 (2012).
90. Zhu Q., Oganov A.R., Glass C.W., Stokes H.T. Structure prediction for molecular crystals using evolutionary algorithms: methodology and applications. *Acta Cryst. B* **68**, 215–226 (2012).
89. Boulfelfel S.E., Oganov A.R., Leoni S. Understanding the nature of “superhard graphite”. *Sci. Rep.* **2**, 471 (2012).
88. Zhong Y., Zhou H.Y., Hu C.-H., Wang D.-H., Oganov A.R. Theoretical study on high-pressure phases, electronic structure, and vibrational properties of $NaNH_2$. *J. Phys. Chem. C* **116**, 8387–8393 (2012).
87. Zhu Q., Oganov A.R., Lyakhov A.O. Evolutionary metadynamics: a novel method to predict crystal structures. *Cryst. Eng. Comm.* **14**, 3596–3601 (2012).
86. Bazhanova Z.G., Oganov A.R., Gianola O. Fe-C-H system at pressures of the Earth’s inner core. *Physics-Uspexhi* **55**, 489–497 (2012).
85. Shirako Y., Kojitani H., Oganov A.R., Fujino K., Miura H., Mori D., Inaguma Y., Yamaura K., Akaogi M. Crystal structure of $CaRhO_3$ polymorph: High-pressure intermediate phase between perovskite and post-perovskite. *Am. Mineral.* **97**, 159–163 (2012).
84. Zhou X.-F., Dong X., Zhao Z., Oganov A.R., Tian Y., Wang H.-T. High-pressure phases of $NaAlH_4$ from

first principles. *Appl. Phys. Lett.* **100**, 061905 (2012).

83. Oganov A.R., Solozhenko V.L., Gatti C., Kurakevych O.O., Le Godec Y. The high-pressure phase of boron, γ -B₂₈: disputes and conclusions of 5 years after discovery. *J. Superhard Materials* **33**, 363–379 (2011).

82. Lyakhov A.O., Oganov A.R. Evolutionary search for superhard materials applied to forms of carbon and TiO₂. *Phys. Rev. B* **84**, 092103 (2011).

81. Zhou X.-F., Oganov A.R., Dong X., Zhang L., Tian Y., Wang H.-T. Superconducting high pressure phase of platinum hydride. *Phys. Rev. B* **84**, 054543 (2011).

80. Zhu Q., Oganov A.R., Salvado M., Pertierra P., Lyakhov A.O. Denser than diamond: ab initio search for superdense carbon allotropes. *Phys. Rev. B* **83**, 193410 (2011).

79. Wen X.D., Hand L., Labet V., Yang T., Hoffmann R., Ashcroft N.W., Oganov A.R., Lyakhov A.O. Graphane sheets and crystals under pressure. *Proc. Natl. Acad. Sci.* **108**, 6833–6837 (2011).

78. Oganov A.R., Lyakhov A.O., Valle M. How evolutionary crystal structure prediction works - and why. *Acc. Chem. Res.* **44**, 227–237 (2011).

77. Oganov A.R., Ma Y., Lyakhov A.O., Valle M., Gatti C. Evolutionary crystal structure prediction as a method for the discovery of minerals and materials. *Rev. Mineral. Geochem.* **71**, 271–298 (2010).

76. Gao G., Oganov A.R., Wang H., Li P., Ma Y., Cui T., Zou G. Dissociation of methane under high pressure. *J. Chem. Phys.* **133**, 144508 (2010).

75. Valle M., Oganov A.R. Crystal fingerprints space. A novel paradigm to study crystal structures sets. *Acta Cryst. A* **66**, 507–517 (2010).

74. Lyakhov A.O., Oganov A.R., Valle M. How to predict very large and complex crystal structures. *Comp. Phys. Comm.* **181**, 1623–1632 (2010).

73. Oganov A.R., Lyakhov A.O. Towards the theory of hardness of materials. *J. Superhard Mater.* **32**, 143–147 (2010).

72. Jung D.Y., Vinograd V.L., Fabrichnaya O.B., Oganov A.R., Schmidt M.W., Winkler B. Thermodynamics of mixing in MgSiO₃-Al₂O₃ perovskite and ilmenite from ab initio calculations. *Earth Planet. Sci. Lett.* **295**, 477–486 (2010).

71. Xie Y., Oganov A.R., Ma Y. Novel structures and high pressure superconductivity of CaLi₂. *Phys. Rev. Lett.* **104**, 177005 (2010).

70. Oganov A.R., Ma Y.M., Xu Y., Errea I., Bergara A., Lyakhov A.O. Exotic behavior and crystal structures of calcium under pressure. *Proc. Natl. Acad. Sci.* **107**, 7646–7651 (2010).

69. Gao G., Oganov A.R., Li Z., Li P., Cui T., Bergara A., Lyakhov A.O., Ma Y., Iitaka T., Zou G. Crystal structures and superconductivity of stannane under high pressure. *Proc. Natl. Acad. Sci.* **107**, 1317–1320 (2010).

68. Zhang F., Oganov A.R. Iron silicides at pressures of the Earth's inner core. *Geophys. Res. Lett.* **37**, L02305 (2010).

67. Zurek E., Hoffmann R., Ashcroft N.W., Oganov A.R., Lyakhov A.O. A little bit of lithium does a lot for hydrogen. *Proc. Natl. Acad. Sci.* **106**, 17640–17643 (2009).

66. Oganov A.R., Solozhenko V.L. Boron: a hunt for superhard polymorphs. *J. Superhard Materials* **31**, 285–291 (2009).

65. Hu C.H., Oganov A.R., Lyakhov A.O., Zhou H.Y., Hafner J. Insulating states of LiBeH₃ under extreme compression. *Phys. Rev. B* **79**, 134116 (2009).

64. Li Q., Ma Y., Oganov A.R., Wang H.B., Wang H., Xu Y., Cui T., Mao H.-K., Zou G. Superhard monoclinic polymorph of carbon. *Phys. Rev. Lett.* **102**, 175506 (2009).

63. Wang H., Li Q., Li Y., Cui T., Oganov A.R., Ma Y. Ultra-incompressible phases of tungsten dinitride predicted from first principles. *Phys. Rev. B* **79**, 132109 (2009).

62. Schönborn S., Goedecker S., Roy S., Oganov A.R. The performance of minima hopping and evolutionary algorithms for cluster structure prediction. *J. Chem. Phys.* **130**, 144108 (2009).

61. Xu Y., Tse J.S., Oganov A.R., Cui T., Wang H., Ma Y., Zou G. Superconducting high-pressure phase of cesium iodide. *Phys. Rev. B* **79**, 144110 (2009).

60. Li Q., Wang M., Oganov A.R., Cui T., Ma Y., Zou G. Rhombohedral superhard structure of BC₂N. *J. Appl. Phys.* **105**, 053514 (2009).

59. Oganov A.R., Valle M. How to quantify energy landscapes of solids. *J. Chem. Phys.* **130**, 104504 (2009).

58. Ma Y., Eremets M.I., Oganov A.R., Xie Y., Trojan I., Medvedev S., Lyakhov A.O., Valle M., Prakapenka V. Transparent dense sodium. *Nature* **458**, 182–185 (2009).
57. Martinez-Canales M., Oganov A.R., Lyakhov A., Ma Y., Bergara A. Novel structures of silane under pressure. *Phys. Rev. Lett.* **102**, 087005 (2009).
56. Ma Y., Oganov A.R., Xie Y., Li Z., Kotakoski J. Novel high pressure structures of polymeric nitrogen. *Phys. Rev. Lett.* **102**, 065501 (2009).
55. Ma Y., Wang Y., Oganov A.R. Absence of superconductivity in the novel high-pressure polymorph of MgB_2 . *Phys. Rev. B* **79**, 054101 (2009).
54. Oganov A.R., Chen J., Gatti C., Ma Y.-Z., Ma Y.-M., Glass C.W., Liu Z., Yu T., Kurakevych O.O., Solozhenko V.L. Ionic high-pressure form of elemental boron. *Nature* **457**, 863–867 (2009).
53. Solozhenko V.L., Kurakevych O.O., Oganov A.R. On the hardness of a new boron phase, orthorhombic $\gamma\text{-B}_{28}$. *J. Superhard Mater.* **30**, 428–429 (2008).
52. Errea I., Martinez-Canales M., Oganov A.R., Bergara A. Fermi surface nesting and phonon instabilities in simple cubic calcium. *High Press. Res.* **28**, 443–448 (2008).
51. Hu C.H., Oganov A.R., Wang Y.M., Zhou H.Y., Lyakhov A., Hafner J. Crystal structure prediction of LiBeH_3 using ab initio total-energy calculations and evolutionary simulations. *J. Chem. Phys.* **129**, 234105 (2008).
50. Valle M., Oganov A.R. Crystal structure classifier for an evolutionary algorithm structure predictor. *IEEE Symposium on Visual Analytics Science and Technology (October 21 - 23, Columbus, Ohio, USA), pp. 11–18 (2008).
49. Gao G., Oganov A.R., Bergara A., Martinez-Canalez M., Cui T., Iitaka T., Ma Y., Zou G. Superconducting high pressure phase of germane. *Phys. Rev. Lett.* **101**, 107002 (2008).
48. Oganov A.R., Ono S., Ma Y., Glass C.W., Garcia A. Novel high-pressure structures of MgCO_3 , CaCO_3 and CO_2 and their role in the Earth's lower mantle. *Earth Planet. Sci. Lett.* **273**, 38–47 (2008).
47. Ma Y., Oganov A.R., Xie Y. High pressure structures of lithium, potassium, and rubidium predicted by ab initio evolutionary algorithm. *Phys. Rev. B* **78**, 014102 (2008).
46. Ono S., Oganov A.R., Brodholt J.P., Voadlo L., Wood I.G., Lyakhov A., Glass C.W., Côté A.S., Price G.D. High-pressure phase transformations of FeS: novel phases at conditions of planetary cores. *Earth Planet. Sci. Lett.* **272**, 481–487 (2008).
45. Koci L., Ma Y., Oganov A.R., Souvatzis P., Ahuja R. Anomalous elastic behavior of superconducting metals V, Nb, Ta, Mo, and W at high pressure. *Phys. Rev. B* **77**, 214101 (2008).
44. Oganov A.R., Glass C.W. Evolutionary crystal structure prediction as a tool in materials design. *J. Phys.: Cond. Matter* **20**, 064210 (2008).
43. Martoňák R., Donadio D., Oganov A.R., Parrinello M. 4- to 6- coordinated silica: transformation pathways from metadynamics. *Phys. Rev. B* **76**, 014120 (2007).
42. Ma Y.-M., Oganov A.R., Glass C.W. Structure of the metallic ζ -phase of oxygen and isosymmetric nature of the ε - ζ phase transition: Ab initio simulations. *Phys. Rev. B* **76**, 064101 (2007).
41. Martoňák R., Oganov A.R., Glass C.W. Crystal structure prediction and simulations of structural transformations: metadynamics and evolutionary algorithms. *Phase Transitions* **80**, 277–298 (2007).
40. Hassdenteufel K.H., Oganov A.R., Steurer W., Katrich S. Ab initio study of the W-phase of Al-Co-Ni, an approximant of the decagonal Al-Co-Ni quasicrystal. *Phys. Rev. B* **75**, 144115 (2007).
39. Xie Y., Tse J.S., Oganov A.R., Cui T., Zou G. Electronic and phonon instabilities in face-centered cubic alkali metals under pressure. *Phys. Rev. B* **75**, 064102 (2007).
38. Dorogokupets P.I., Oganov A.R. Ruby, metals, and MgO as alternative pressure scales: A semiempirical description of shock-wave, ultrasonic, x-ray, and thermochemical data at high temperatures and pressures. *Phys. Rev. B* **75**, 024115 (2007).
37. Glass C.W., Oganov A.R., Hansen N. USPEX – evolutionary crystal structure prediction. *Comp. Phys. Comm.* **175**, 713–720 (2006).
36. Zhang F., Oganov A.R. Valence and spin states of iron impurities in mantle-forming silicates. *Earth Planet. Sci. Lett.* **249**, 436–443 (2006).
35. Pushcharovsky D.Yu., Oganov A.R. Structural transformations of minerals in deep geospheres: a review. *Crystallography Rep.* **51**, 767–777 (2006).
34. Dorogokupets P.I., Oganov A.R. Equations of state of Al, Au, Cu, Pt, Ta and W and the revised ruby pressure scale. *Doklady Earth Sciences* **410**, 1091–1095 (2006).

- 33. Martoňák R., Donadio D., Oganov A.R., Parrinello M.** Crystal structure transformations in SiO₂ from classical and ab initio metadynamics. *Nature Mater.* **5**, 623–626 (2006).
- 32. Oganov A.R., Glass C.W.** Crystal structure prediction using ab initio evolutionary techniques: principles and applications. *J. Chem. Phys.* **124**, 244704 (2006).
- 31. Zhang F., Oganov A.R.** Mechanisms of Al³⁺ incorporation in MgSiO₃ post-perovskite at high pressures. *Earth Planet. Sci. Lett.* **248**, 54–61 (2006).
- 30. Ono S., Oganov A.R., Koyama T., Shimizu H.** Stability and compressibility of high-pressure phase of Al₂O₃ up to 200 GPa: implications for electrical conductivity at the base of the lower mantle. *Earth Planet. Sci. Lett.* **246**, 326–335 (2006).
- 29. Adams D.J., Oganov A.R.** Ab initio molecular dynamics study of CaSiO₃ perovskite at P-T conditions of Earth's lower mantle. *Phys. Rev. B* **73**, 184106 (2006).
- 28. Boldyreva E.V., Ahsbahs H., Chernyshev V.V., Ivashevskaya S.N., Oganov A.R.** Effect of hydrostatic pressure on the crystal structure of sodium oxalate: X-ray diffraction study and ab initio simulations. *Z. Krist.* **221**, 186–197 (2006).
- 27. Ghose S., Krisch M., Oganov A.R., Beraud A., Bossak A., Gulve R., Seelaboyina R., Yang H., Saxena S.K.** Lattice dynamics of MgO at high pressure: theory and experiment. *Phys. Rev. Lett.* **96**, 035507 (2006).
- 26. Oganov A.R., Glass C.W., Ono S.** High-pressure phases of CaCO₃: crystal structure prediction and experiment. *Earth Planet. Sci. Lett.* **241**, 95–103 (2006).
- 25. Oganov A.R., Martoňák R., Laio A., Raiteri P., Parrinello M.** Anisotropy of Earth's D'' layer and stacking faults in the MgSiO₃ post-perovskite phase. *Nature* **438**, 1142–1144 (2005).
- 24. Oganov A.R., S. Ono** The high-pressure phase of alumina and implications for Earth's D'' layer. *Proc. Natl. Acad. Sci.* **102**, 10828–10831 (2005).
- 23. Ono S., Oganov A.R.** In situ observations of phase transition between perovskite and CaIrO₃-type phase in MgSiO₃ and pyrolitic mantle composition. *Earth Planet. Sci. Lett.* **236**, 914–932 (2005).
- 22. Jung D.Y., Oganov A.R.** Ab initio study of the high-pressure behaviour of CaSiO₃ perovskite. *Phys. Chem. Minerals* **32**, 146–153 (2005).
- 21. Oganov A.R., Price G.D., Scandolo S.** Ab initio theory of planetary materials. *Z. Krist.* **220**, 531–548 (2005).
- 20. Oganov A.R., Price G.D.** Ab initio thermodynamics of MgSiO₃ perovskite at high pressures and temperatures. *J. Chem. Phys.* **122**, 124501 (2005).
- 19. Alfredsson M., Dobson D.P., Oganov A.R., Catlow C.R.A., Brodholt J.P., Parker S.C., Price G.D.** Crystal morphology and surface structures of the orthorhombic MgSiO₃ perovskite. *Phys. Chem. Minerals* **31**, 671–682 (2005).
- 18. Oganov A.R., Gillan M.J., Price G.D.** Structural stability of silica at high pressures and temperatures. *Phys. Rev. B* **71**, 064104 (2005).
- 17. Oganov A.R., Ono S.** Theoretical and experimental evidence for a post-perovskite phase of MgSiO₃ in Earth's D'' layer. *Nature* **430**, 445–448 (2004).
- 16. Oganov A.R. & Dorogokupets P.I.** Intrinsic anharmonicity in thermodynamics and equations of state of solids. *J. Phys.: Cond. Matter.* **16**, 1351–1360 (2004).
- 15. Dorogokupets P.I. & Oganov A.R.** Intrinsic anharmonicity in equations of state of solids and minerals. *Doklady Earth Sciences* **395**, 238–241 (2004).
- 14. Senyshyn A., Oganov A.R., Vasylechko L., Ehrenberg H., Bismayer U., Berkowski M., Matkovskii A.** Crystal structure and thermal expansion of the perovskite – type Nd_{0.75}Sm_{0.25}GaO₃ – powder diffraction and lattice dynamical studies. *J. Phys.: Cond. Matter.* **16**, 253–265 (2004).
- 13. Dorogokupets P.I. & Oganov A.R.** Equations of state of Cu and Ag and the revised ruby pressure scale. *Doklady Earth Sciences* **391A**, 854–857 (2003).
- 12. Oganov A.R. & Dorogokupets P.I.** All-electron and pseudopotential study of MgO: Equation of state, anharmonicity, and stability. *Phys. Rev. B* **67**, 224110 (2003).
- 11. Oganov A.R., Gillan M.J., Price G.D.** Ab initio lattice dynamics and structural stability of MgO. *J. Chem. Phys.* **118**, 10174–10182 (2003).
- 10. Brodholt J.P., Oganov A.R., Price G.D.** Computational mineral physics and physical properties of perovskite. *Phil. Trans. Royal Soc. London A* **360**, 2507–2520 (2002).
- 9. Oganov A.R., Price G.D., Brodholt J.P.** Theoretical investigation of metastable Al₂SiO₅

polymorphs. *Acta Crystallogr. A* **57**, 548–557 (2001).

8. Oganov A.R., Brodholt J.P., Price G.D. The elastic constants of MgSiO_3 perovskite at pressures and temperatures of the Earth's mantle. *Nature* **411**, 934–937 (2001).

7. Oganov A.R., Brodholt J.P., Price G.D. Ab initio elasticity and thermal equation of state of MgSiO_3 perovskite. *Earth and Planetary Science Letters* **184**, 555–560 (2001).

6. Oganov A.R., Organova N.I., Urusov V.S. Nature of Al-Si anti-ordering in a two-phase feldspar from the Pektusan volcano. *Geochem. Int.* **39**, 1160–1171 (2001).

5. Oganov A.R., Brodholt J.P., Price G.D. Comparative study of quasiharmonic lattice dynamics, molecular dynamics and Debye model in application to MgSiO_3 perovskite. *Phys. Earth Planet. Int.* **122**, 277–288 (2000).

4. Oganov A.R., and Brodholt J.P. High-pressure phases in the Al_2SiO_5 system and the problem of Al-phase in Earth's lower mantle: ab initio calculations. *Phys. Chem. Minerals* **27**, 430–439 (2000).

3. Urusov V.S., Eremin N.N., Oganov A.R. Modeling of structures and properties of oxide crystals by minimization of the atomization energy. *Crystallography Rep.* **44**, 356–365 (1999).

2. Urusov V.S., Oganov A.R., Eremin N.N. Computer simulation of structure, properties and stability of Al_2SiO_5 polymorphs. I. Ionic approximation. *Geochem. Int.* **36**, 397–414 (1998).

1. Oganov A.R. A finding of rhombohedral pyrite crystals. *Proc. Russ. Min. Soc.*, No.1, 65–69 (1996).