

Professor Artem R. Oganov FRSC MAE

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ADDRESS: Skolkovo Institute of Science and Technology, Bolshoy Boulevard 30, bld. 1, 121205 Moscow, Russia. E-mail: a.oganov@skoltech.ru. Telephone: +7-(495)-240-1481.

DATE OF BIRTH: 03.03.1975.

PERSONAL INFORMATION: Married, four children (daughters Jeanne and Adriana, sons Lev and Alexander). Speaks five languages (native Russian, fluent English, intermediate French, basic Italian and German).

PROFESSIONAL EXPERIENCE AND EDUCATION:

06/2024-now : Distinguished Professor, Skolkovo Institute of Science and Technology, Russia.
 2015-06/2024 : 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 (in 2021-2024 Head of Department of Semiconductors and Dielectrics).
 2017 : Founded and directed (until 2020) the 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), Dept. Geosciences & Institute for Advanced Computational Sciences, Stony Brook University, U.S.A.
 2007 : Habilitation, Dept. Materials, ETH Zurich, Switzerland - in 2016 accepted as equivalent to Doctor of Physical & Mathematical Sciences (Russian highest degree)
 2003-2008 : Senior scientist (2003-2007) and Privatdozent (2007-2008), Dept. Materials, ETH Zurich, Switzerland
 2002-2003 : Research Fellow, University College London, U.K.
 2002 : PhD in Crystallography, University College London, U.K.
 1997 : M.Sc. in Crystallography, Moscow State University, *magna summa cum laude*.

PUBLICATIONS: 348 papers (including 5 in *Nature* and 2 in *Science*) and book chapters.

Web of Science: total citation = 27,187, h-index = 80.

Google Scholar: total citation = 37,307, h-index = 90.

Author and coauthor of three scientific books and one best-selling popular science book.

INVITED LECTURES: 532 talks at universities and conferences, including 83 plenary and keynote lectures.

VISITING APPOINTMENTS: Adjunct Professor of Moscow State University since 2006 and Northwestern Polytechnical University (China) since 2012. Since 2005 was an invited professor in Italy (Milan), France (Paris, Lille and Poitiers), China (Guilin, Beijing, Hong Kong, Kaifeng, Urumqi).

MAJOR DISTINCTIONS:

2024 : Elected Distinguished Professor of Skolkovo Institute of Science and Technology
 2024 : Tianshan Award for Foreign Experts (Xinjiang Province, China)
 2024 : Distinguished Scientist of the President's International Fellow Initiative (PIFI), Chinese Academy of Sciences.
 2024 : Fellow of the International Core Academy of Sciences and Humanities
 2024 : Znanie Award in two nominations (1 - for popularizing science and technologies, 2 – for general contribution to education)
 2023 : "For the commitment to science" National Award for popularization of science
 2022 : Highly Cited Researcher by Clarivate Analytics (0.1% most cited researchers)
 2020 : Fellow of the American Physical Society
 2020 : Fellow of the Royal Society of Chemistry (FRSC)
 2019- : every year after 2019 ranked in top 2% most cited scientists (Elsevier)
 2019 : Friendship award of Chinese government
 2017 : George Gamow award
 2017 : Concord award
 2017 : Member of Academia Europaea (M.A.E.)
 2017 : Russian Highly Cited Researcher in Physics (Clarivate Analytics)
 2017 : Chinese Academy of Sciences Presidential Visiting Fellowship
 2017 : Paper (*J. Chem. Phys.* 2006) declared citation classic by Google Scholar

- 2016 : Russian Highly Cited Researcher award (Chemistry), by Clarivate Analytics
 2015 : Japan Society for Promotion of Science Invitation Fellow
 2015 : Professor of Russian Academy of Sciences
 2013 : Fellow of the Mineralogical Society of America
 2013 : Megagrant of Russian government
 2012 : 1000 talents professor of People's Republic of China
 2012 : Honorary Professor, Yanshan University, China
 2007 : Research Excellence Medal of the European Mineralogical Union
 2006 : University Latsis Prize
 2004 : European High-Pressure Research Group Award
 2003 : Young Scientist Award of the European Union of Geosciences
 2002 : President's Award of the Geological Society of London

IN MEDIA: Ranked among the most successful Russian scientists by Russian Newsweek (2008), Forbes Russia (2011), and Russian Reporter magazine (2014). Ranked among the most influential Russians by GQ (2019).

Participated in films about science and scientists: "Watching the thought fly" (directed by V. Gerchikov, 2017), "New element in the Russian table" (directed by E. Tukhareli, 2019).

Biographical and documentary films about Artem R. Oganov:

- "Color of the crystal" (directed by V. Gerchikov, 2012),
 "Made by Russians" (directed by L. Parfenov, 2015),
 "House of science: Artem Oganov" (directed by N. Popova, 2018),
 "Cool story: Return of the professor" (directed by T. Mitkova, 2018).

SELECT PROFESSIONAL SERVICES:

- 2024-now : Executive editor of chemistry and editorial board member, The Innovation (impact factor >30).
 2023-now : Chairman, Scientific Council, National Science and Technology Prize "Vyzov" ("Challenge")
 2021-now : Editorial Board (Chemistry section) of Russian Encyclopedia
 2021-now : Science and Technology Council, Rusnano Corporation
 2021-now : Academic Council, MISIS University, Russia
 2021-now : Academic Council for Materials and Nanomaterials, Russian Academy of Sciences
 2021-2023 : Academic Council for Geochemistry Problems, Russian Academy of Sciences
 2019-now : Academic Council for Chemical Physics, Russian Academy of Sciences
 2019-2023 : Academic Council, Russian Railways Corporation
 2017-2020 : Member of Russian Presidential Council for Science and Education
 2017-2023 : Consultant, Commission on Crystallography of Materials of IUCr
 2017 : Co-chairman of two panels at World Economic Forum (Dalian, June 2017)
 2017 : Award Committee, RusnanoPrize
 2016-now : Academic Council, Fersman Mineralogical Museum
 2016-2019 : Academic Council, Skolkovo Institute of Science and Technology
 2011-2017 : Founder and Chairman, Commission on Crystallography of Materials of IUCr
 2011-2022 : Organized 21 workshops on crystal structure prediction in France, China, India, Canada, USA, Switzerland, Italy, Iran, Russia.
 2010-now : Member of program and scientific advisory committees of several international conferences, e.g., the International Union of Crystallography (IUCr) meeting, Montreal, August 2014.
 2009-2012 : Member of the University Senate, Stony Brook University.
 2006-now : member of editorial boards of *Scientific Reports* (2006-now), *Journal of Superhard Materials* (2009-now), *Geochemistry International* (2021-), Associate Editor of *American Mineralogist* (2006-2010), *Crystals* (2020-), *Geochemistry International* (2021-).
 2005-2014 : Organized 6 highly cited special issues: "Computational Crystallography" (*Zeitschrift fuer Kristallographie*, 2005); "Computational Materials Discovery" (*Acta Crystallographica.C*, 2014); Special issues of the *Journal of Superhard Materials*: "Theory of Superhard Materials" (2010), "Boron and Boron-rich Solids" (2011), "Superhard Carbon" (2012), "Novel Superhard Materials" (2014).
 2005-now : referee for >60 journals (including *Nature*, *Science*; *Nature Chemistry*, *Nature Materials*; *Nature Geoscience*; *PNAS*, *Phys. Rev. Lett.*, etc.) and for numerous funding agencies around the world.

PROFESSORS TRAINED:

- Yanming Ma (was my postdoc in 2006-2008, now Academician of Chinese Academy of Sciences).
 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 Assoc. Prof. at Nankai U., China).
Qingfeng Zeng (visiting scientist in 2011-2012, now Assoc. Prof., Northwestern Polytechnical U., China).
Chao hao 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 Full Professor at Skoltech).
Congwei Xie (PhD student in 2015-2019, now Assistant Professor at Xinjiang Technical Institute of Physics and Chemistry, China).

PHD STUDENTS GRADUATED:

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 Feyta (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).

DSC THESIS SUPERVISED:

Alexander Kvashnin (2021).

List of publications of Artem R. Oganov.

BOOKS:

4. Oganov A.R. *Chemistry*. AST Publishing House. Moscow. (popular science book, in Russian). ISBN 978-5-17-145181-3. (2022).
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. (in Russian). ISSN 2686-9993. (2021).
2. Oganov A.R., Saleh G., Kvashnin A.G. (Editors). *Computational Materials Discovery*. Royal Society of Chemistry. ISBN: 978-1-78262-961-0. (2018).
1. Oganov A.R. (Editor). *Modern Methods of Crystal Structure Prediction*. Berlin: Wiley-VCH. ISBN: 978-3-527-40939-6. (2010).

REVIEWS AND CHAPTERS IN BOOKS:

21. Oganov A.R., Konson G.R. (2020). 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.
20. Kruglov I.A., Dolgirev P.E., Oganov A.R., Mazitov A.B., Pozdnyakov S.N., Mazhnik E.A., Yanilkin A.V. (2019). Machine leaning 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.
19. Allahyari Z., Oganov A.R. (2018). 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.
18. Oganov A.R., Kvashnin A.G., Saleh G. (2018). Computational materials discovery: dream or reality? In: *Computational Materials Discovery*. Eds.: Oganov A.R., Kvashnin A.G., Saleh G. Royal Society of Chemistry, pp. 1-14.
17. Oganov A.R., Kruglov I.A., Zhang J., Davari Esfahani M. (2018). Computational materials discovery using evolutionary algorithms. In: *Computational Materials Discovery*. Eds.: Oganov A.R., Kvashnin A.G., Saleh G. Royal Society of Chemistry, pp. 15-65.
16. Dong X., Oganov A.R. (2017). 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.
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. (2017). Predicting the structure and chemistry of low-dimensional materials. *Handbook of Solid State Chemistry*, v.5, eds. R. Dronskowski, S. Kikkawa, A. Stein. Pp. 527-570.
14. Oganov A.R., Lyakhov A.O., Zhu Q. (2014). Theory of superhard materials. In: *Comprehensive Hard Materials Review*, Elsevier, v.3, 59-79.
13. Oganov A.R. (2011). 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.
12. Oganov A.R. (2011). 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.
11. Oganov A.R., Schön J.C., Jansen M., Woodley S.M., Tipton W.W., Hennig R.G. (2010). 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.
10. Lyakhov A.O., Oganov A.R., Valle M. (2010). Crystal structure prediction using evolutionary approach. In: *Modern methods of crystal structure prediction* (ed. A.R. Oganov), pp. 147-180. Berlin: Wiley-VCH.
9. Oganov A.R. (2010). Crystal structure prediction, a formidable problem. In: *Modern Methods of Crystal Structure Prediction* (ed. A.R. Oganov), pp. xi-xxi. Berlin: Wiley-VCH.
8. Oganov A.R., Ma Y., Lyakhov A.O., Valle M., Gatti C. (2010). Evolutionary crystal structure prediction and novel high-pressure phases. "High-pressure crystallography" (eds. E. Boldyreva, P. Dera), pp. 293-325. Springer Verlag.
7. Oganov A.R., Ma Y., Glass C.W., Valle M. (2007). Evolutionary crystal structure prediction: overview of the USPEX method and some of its applications. *Psi-k Newsletter*, number **84**, Highlight of the Month, 142-171 (invited review).
6. Oganov A.R. (2007). 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), 121-152.
5. Jung D.Y., Oganov A.R. (2005). Basics of first-principles simulation of matter under extreme conditions. *EMU Notes in Mineralogy v.7* ("High-Pressure Behaviour of Minerals", edited by R. Miletich), 117-138.
4. Adams D.J., Oganov A.R. (2005). Theory of minerals at extreme conditions: predictability of structures and properties. *EMU Notes in Mineralogy v.7* ("High-Pressure Behaviour of Minerals", edited by R. Miletich), 441-457.

3. Oganov A.R. (2004). 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.
2. Oganov A.R. (2003). 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, p.199-215 (edited by A.Katrusiak, P.F.McMillan). Kluwer Academic Publishers, Dordrecht.
1. Oganov A.R., Brodholt J.P., Price G.D. (2002). Ab initio theory of thermoelasticity and phase transitions in minerals. *EMU Notes in Mineralogy* v.4 ('Energy Modelling in Minerals', edited by C.M. Gramaccioli), pp.83-170.

PAPERS IN REFEREED JOURNALS

327. Fedyaeva M., Lepeshkin S.V., Chukanov N.V., Oganov A.R. (2024). Mutual transformations of polysulfide chromophore species in sodalite-group minerals: a DFT study of S₆ decomposition. *ChemPhysChem*, art. e202400532.
326. Jalolov F.N., Podryabinkin E.V., Oganov A.R., Shapeev A.V., Kvashnin A.G. (2024). Mechanical properties of single and polycrystalline solids from machine learning. *Adv. Theory and Simul.* **7**, 2301171.
325. Novoselov D.Yu., Korotin D.M., Shorikov A.O., Anisimov V.I., Oganov A.R. (2024). Electronic correlations and intrinsic magnetism of interstitial quasi-atomic states in Li₈Au electride. *Phys. Chem. Chem. Phys.* **26**, 17854-17859.
324. Zhou D., Semenok D., Galasso M., Alabarse F.G., Sannikov D., Troyan I.A., Nakamoto Y., Shimizu K., Oganov A.R. (2024). Raisins in a hydrogen pie: ultrastable cesium and rubidium polyhydrides. *Adv. Energy Mater.* **14**, 2400077.
323. Anisimov V.I., Oganov A.R., Korotin D.M., Novoselov D.Y., Shorikov A.O., Belozerov A.S. (2024). First-principles definition of ionicity and covalency in molecules and solids. *J. Chem. Phys.* **160**, 144113.
322. Banaru D.A., Aksenov S.M., Banaru A.M., Oganov A.R. (2024). Mutual correlations of complexity indices of the crystal structure for the series of mercury-containing minerals. *Z. Krist.*, <https://doi.org/10.1515/zkri-2024-0062>
321. Iosimovska A.V., Maltsev A.P., Chepkasov I.V., Oganov A.R. (2024). Thermodynamic stability and ionic conductivity in lithium-germanium binary system. *Appl. Phys. Lett.* **124**, 163904.
320. Zeraati M., Oganov A.R., Fan T., Solodovnikov S.F. (2024). Searching for low thermal conductivity materials for thermal barrier coatings: A theoretical approach. *Phys. Rev. Materials* **8**, 033601.
319. Chepkasov I.V., Kvashnin A.G., Radina A.D., Matsokin N.A., Jalolov F.N., Oganov A.R., Dashevsky Z. (2024). Origin of brittle behavior of doped PbTe-based thermoelectric materials. *Appl. Phys. Lett.* **124**, 022104.
318. Maltsev A.P., Chepkasov I.V., Oganov A.R. (2024). New promising class of anode materials for Ca-ion battery: Polyaromatic hydrocarbons. *Materials Today Energy* **39**, 101467.
317. Shutov G.M., Semenok D.V., Kruglov I.A., Oganov A.R. (2024). Ternary superconducting hydrides in the La–Mg–H system. *Materials Today Physics* **40**, 101300.
316. Korotin D.M., Novoselov D.Y., Shorikov A.O., Anisimov V.I., Oganov A.R. (2023). Electronic correlations in the ultranarrow energy band compound Pb₉Cu(PO₄)₆O: A DFT+DMFT study. *Phys. Rev.* **B108**, L241111.
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. (2023). Superconductivity in compounds of sodium-intercalated graphite. *Phys. Rev.* **B108**, 214507.
314. Novoselov D.Y., Mazannikova M.A., Korotin D.M., Shorikov A.O., Anisimov V.I., Oganov A.R. (2023). Exploring correlation effects and volume collapse during electride dimensionality change in Ca₂N. *Phys. Chem. Chem. Phys.* **25**, 30960-30965.
313. Mazannikova M.A., Korotin D.M., Anisimov V.I., Oganov A.R., Novoselov D.Y. (2023). Dimensionality-Driven Evolution of Electronic Structure and Transport Properties in Pressure-Induced Phases of Ca₂N Electride. *JETP Lett.* **118**, 651-657.
312. Kruglov I.A., Yanilkin A.V., Propad Y., Mazitov A.B., Rachitskii P., Oganov A.R. (2023). Crystal structure prediction at finite temperatures. *npj Comput. Mater.* **9**, 197.
311. Vaneeva E.E., Lepeshkin S.V., Oganov A.R. (2023). Prediction and Rationalization of Abundant C–N–H Molecules in Different Environments. *J. Phys. Chem. Lett.* **14**, 8367–8375.
310. Maltsev A.P., Chepkasov I.V., Oganov A.R. (2023). Order–Disorder Phase Transition and Ionic Conductivity in a Li₂B₁₂H₁₂ Solid Electrolyte. *ACS Appl. Mater. Interfaces* **15**, 42511–42519.
309. Mikhailova A.A., Lepeshkin S.V., Baturin V.S., Maltsev A.P., Uspenskii Y.A., Oganov A.R. (2023). Ultralow reaction barriers for CO oxidation in Cu–Au nanoclusters. *Nanoscale* **15**, 13699-13707.
308. Huang H.-M., Zhu Q., Blatov V.A., Oganov A.R., Wei H., Jiang P., Li Y.-L. (2023). Novel Topological Motifs and Superconductivity in Li-Cs System. *Nano Lett.* **23**, 5012-5018.
307. Chen W., Huang X., Semenok D.V., Chen S., Zhang K., Oganov A.R., Cui T. (2023). Enhancement of the superconducting critical temperature realized in the La-Ce-H system at moderate pressures. *Nature Communications* **14**, 2660.

306. Maltsev A.P., Chepkasov I.V., Kvashnin A.G., Oganov A.R. (2023). Ionic conductivity of lithium phosphides. *Crystals* **13**, 756.
305. Pozdnyakov S., Oganov A.R., Mazhnik E., Mazitov A., Kruglov I. (2023). Fast general two- and three-body interatomic potential. *Phys. Rev.* **B107**, 125160.
304. Fedyaeva M., Lepeshkin S., Oganov A.R. (2023). Stability of sulfur molecules and insights into sulfur allotropy. *Phys. Chem. Chem. Phys.* **25**, 9294-9299.
303. Anisimov V.I., Oganov A.R., Mazannikova M.A., Novoselov D.Yu., Korotin D.M. (2023). Formal Valence, Charge Distribution and Chemical Bond in a Compound with a High Oxidation State: KMnO_4 . *JETP Lett.* **117**, 377-383.
302. Rachitskii P., Kruglov I., Finkelstein A.V., Oganov A.R. (2023). Protein structure prediction using the evolutionary algorithm USPEX. *Proteins* **2023**, 1-11.
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. (2023). Synthesis of technetium hydride $\text{TcH}_{1.3}$ at 27 GPa. *Phys. Rev.* **B107**, 064102.
300. Rybkovskiy D.V., Lepeshkin S.V., Baturin V.S., Mikhailova A.A., Oganov A.R. (2023). Phosphorus nanoclusters and insight into the formation of phosphorus allotropes. *Nanoscale* **15**, 1338-1346.
299. Galasso M., Oganov A.R. (2023). Automag: An automatic workflow software for calculating the ground magnetic state of a given structure and estimating its critical temperature. *Comp. Phys. Comm.* **283**, 108571.
298. Hou J., Dong X., Oganov A.R., Weng X.-J., Hao C.-M., Yang G., Wang H.-T., Zhou X.-F., Tian Y. (2022). Helium-bearing superconductor at high pressure. *Phys. Rev.* **B106**, L220501.
297. Xie C.W., Tudi A., Oganov A.R. (2022). PNO: a promising deep-UV nonlinear optical material with the largest second harmonic generation effect. *Chem. Commun.* **58**, 12491-12494.
296. Marchenko E.A., Oganov A.R., Mazhnik E.A., Eremin N.N. (2022). Stable compounds in the $\text{CaO-Al}_2\text{O}_3$ system at high pressures. *Phys. Chem. Miner.* **49**, art. 44.
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. (2022). High-temperature superconductivity in hydrides. *Physics-Uspexhi* **192**, 799–813.
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., Maksimtsev K., Mukhamadeev A., Chukin A., Korolev A., Mushnikov N., Li H. (2022). Computational prediction of new magnetic materials. *J. Chem. Phys.* **157**, 124704.
293. Rybin N., Chepkasov I., Novoselov D.Y., Anisimov V.I., Oganov A.R. (2022). Prediction of stable silver fluorides. *J. Phys. Chem.* **C126**, 15057–15063.
292. Momenzadeh-Abardeh Z., Salimi A., Oganov A.R. (2022). Crystal structure prediction of N-halide phthalimide compounds: halogen bonding synthons as a touchstone. *CrystEngComm* **24**, 6066-6075.
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. (2022). Effect of magnetic impurities on superconductivity in LaH_{10} . *Adv. Mater.* **34**, 2204038.
290. Lepeshkin S.V., Naumova A.S., Baturin V.S., Oganov A.R. (2022). "Magic" molecules and a new look at chemical diversity of hydrocarbons. *J. Phys. Chem. Lett.* **13**, 7600-7606.
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. (2022). Sr-Doped Molecular Hydrogen: Synthesis and Properties of SrH_{22} . *Adv. Mater.* 2200924.
288. Novoselov D.Y., Mazannikova M.A., Korotin D.M., Shorikov A.O., Korotin M.A., Anisimov V.I., Oganov A.R. (2022). Localization mechanism of interstitial electronic states in electride mayenite. *J. Phys. Chem. Lett.* **13**, 7155-7160.
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