

Structure and Properties of Pseudo-Graphenes. Review

N.D. Abramenko¹, M.A. Rozhkov¹, A.L. Kolesnikova^{1,2} and A.E. Romanov^{1,3}

¹ITMO University, Kronverksky pr. 49, 197101, St. Petersburg, Russia

²Institute for Problems in Mechanical Engineering, RAS, Bolshoj pr. 61, Vas. Ostrov, 199178, St. Petersburg, Russia

³Ioffe Physical-Technical Institute, RAS, Polytechnicheskaya 26, 194021, St. Petersburg, Russia

Received: December 16, 2021

Corresponding author: M.A. Rozhkov

Abstract. In this review, we consider structure and properties of pseudo-graphenes – graphene-like crystals with high density of non-hexagonal (defective or improper) carbon atomic rings. As an introduction, graphene and its properties are briefly described and disclination defects in graphene are considered. Then, numerous articles presenting *graphene allotropes* and *carbon allotropes* are analyzed. As a result, a term *pseudo-graphene* for description of materials with high density of improper carbon atomic rings arranged periodically is proposed and a unified classification of pseudo-graphenes regarding the materials from observed articles is suggested. The material chart is created based on proposed classification and material properties. In this chart, two categories are reviewed separately: sp^2 pseudo-graphenes and non- sp^2 pseudo-graphenes. The analyzed materials are subdivided into semiconductors, metals, semimetals, and superconductors.

ACKNOWLEDGEMENTS

The support of [RSF](#) grant 19-19-00617 is acknowledged.

REFERENCES

- [1] W. Taylor, *Structure and Properties of Diamond*, Nature, 1947, vol. 159, no. 1947, pp. 729–731.
- [2] J. Suparno, D.A. Halim, A. Setiawan, M. Effendy and J. Jamari, *Graphite as Dry Lubricant to Reduce Rail Wheels Wear Level*, Mater. Sci. Forum, 2019, vol. 961, pp. 126–133.
- [3] P. Qian, H. Zhang, J. Chen, Y. Wen, Q. Luo, Z. Liu, D. You and B. Yi, *A Novel Electrode-bipolar Plate Assembly for Vanadium Redox Flow Battery Applications*, J. Power Sources, 2008, vol. 175, no. 1, pp. 613–620.
- [4] M.S. Dresselhaus and G. Dresselhaus, *Fullerenes and Fullerene Derived Solids as Electronic Materials*, Annu. Rev. Mater. Sci., 1995, vol. 25, no. 1, pp. 487–523.

- [5] N. Gupta, S.M. Gupta and S.K. Sharma, *Carbon Nanotubes: Synthesis, Properties and Engineering Applications*, Carbon Letters, 2019, vol. 29, no. 5. pp. 419–447.
- [6] N. Anzar, R. Hasan, M. Tyagi, N. Yadav and J. Narang, *Carbon Nanotube - A Review on Synthesis, Properties and Plethora of Applications in the Field of Biomedical Science*, Sensors International, 2020, vol. 1, art. 100003.
- [7] M.J. Allen, V.C. Tung and R.B. Kaner, *Honeycomb Carbon: A Review of Graphene*, Chem. Rev., 2010, vol. 110, no. 1, pp. 132–145.
- [8] P. Bhattacharya, R. Fornari and H. Kamimura, *Comprehensive Semiconductor Science and Technology* (Elsevier Science, 2011).
- [9] C.A. Brookes and E.J. Brookes, *Diamond in Perspective: a Review of Mechanical Properties of Natural Diamond*, Diam. Relat. Mater., 1991, vol. 1, no. 1, pp. 13–17.
- [10] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, M.I. Katsnelson, I.V. Grigorieva, S.V. Dubonos and A.A. Firsov, *Two-Dimensional Gas of Massless Dirac Fermions in Graphene*, Nature, 2005, vol. 438, no. 7065, pp. 197–200.
- [11] S. Iijima, *Helical Microtubules of Graphitic Carbon*, Nature, 1991, vol. 354, no. 6348, pp. 56–58.
- [12] H.W. Kroto, J.R. Heath, S.C. O'Brien, R.F. Curl and R.E. Smalley, *C₆₀: Buckminster fullerene*, Nature, 1985, vol. 318, pp. 162–163.
- [13] F.L. Coffman, R. Cao, P.A. Pianetta, S. Kapoor, M. Kelly and L.J. Terminello, *Near-Edge X-ray Absorption of Carbon Materials for Determining Bond Hybridization in Mixed sp²/sp³ Bonded Materials*, Appl. Phys. Lett., 1996, vol. 69, no. 4, pp. 568–570.
- [14] H. Kabir, H. Zhu, J. May, K. Hamal, Y. Kan, T. Williams, E. Echeverria, D.N. McIlroy, D. Estrada, P.H. Davis, T. Pandhi, K. Yocham, K. Higginbotham, A. Clearfield and I.F. Cheng, *The sp²-sp³ Carbon Hybridization Content of Nanocrystalline Graphite from Pyrolyzed Vegetable Oil, Comparison of Electrochemistry and Physical Properties with Other Carbon Forms and Allotropes*, Carbon, 2019, vol. 144, pp. 831–840.
- [15] A.H. Castro Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov and A.K. Geim, *The Electronic Properties of Graphene*, Rev. Mod. Phys., 2009, vol. 81, pp. 109–162.
- [16] A.K. Geim and K.S. Novoselov, *The Rise of Graphene*, Nat. Mater., 2007, vol. 6, no. 3, pp. 183–191.
- [17] S. Chen, A.L. Moore, W. Cai, J. W. Suk, J. An, C. Mishra, C. Amos, C.W. Magnuson, J. Kang, L. Shi and R.S. Ruoff, *Raman Measurements of Thermal Transport in Suspended Monolayer Graphene of Variable Sizes in Vacuum and Gaseous Environments*, ACS Nano, 2010, vol. 5, no. 1, pp. 321–328.
- [18] A.A. Balandin, *Thermal Properties of Graphene and Nanostructured Carbon Materials*, Nat. Mater., 2011, vol. 10, no. 8, pp. 569–581.
- [19] S. Chen, Q. Wu, C. Mishra, J. Kang, H. Zhang, K. Cho, W. Cai, A.A. Balandin and R.S. Ruoff, *Thermal Conductivity of Isotopically Modified Graphene*, Nat. Mater., 2012, vol. 11, no. 3, pp. 203–207.
- [20] C. Lee, X. Wei, J.W. Kysar and J. Hone, *Measurement of the Elastic Properties and Intrinsic Strength of Monolayer Graphene*, Science, 2008, vol. 321, no. 5887, pp. 385–388.
- [21] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva and A.A. Firsov, *Electric Field Effect in Atomically Thin Carbon Films*, Science, 2004, vol. 306, no. 5696, pp. 666–669.
- [22] Z.H. Ni, T. Yu, Y.H. Lu, Y.Y. Wang, Y.P. Feng and Z.X. Shen, *Uniaxial Strain on Graphene: Raman Spectroscopy Study and Band-Gap Opening*, ACS Nano, 2008, vol. 2, no. 11, pp. 2301–2305.
- [23] Y.-J. Yu, Y. Zhao, S. Ryu, L.E. Brus, K.S. Kim and P. Kim, *Tuning the Graphene Work Function by Electric Field Effect*, Nano Lett., 2009, vol. 9, no. 10, pp. 3430–3434.
- [24] M.O. Goerbig, *Electronic Properties of Graphene in a Strong Magnetic Field*, Rev. Mod. Phys., 2011, vol. 83, no. 4, pp. 1193–1243.
- [25] F. Hao, D. Fang and Z. Xu, *Mechanical and Thermal Transport Properties of Graphene with Defects*, Appl. Phys. Lett., 2011, vol. 99, no. 4, art. 041901.
- [26] Y. Wei, J. Wu, H. Yin, X. Shi, R. Yang and M. Dresselhaus, *The Nature of Strength Enhancement and Weakening by Pentagon–Heptagon Defects in Graphene*, Nat. Mater., 2012, vol. 11, no. 9, pp. 759–763.

- [27] S.H.M. Jafri, K. Carva, E. Widenkvist, T. Blom, B. Sanyal, J. Fransson, O. Eriksson, U. Jansson, H. Grennberg, O. Karis, R. A. Quinlan, B. C. Holloway and K. Leifer, *Conductivity Engineering of Graphene by Defect Formation*, J. Phys. D: Appl. Phys., 2010, vol. 43, no. 4, art. 045404.
- [28] A. Bagri, S.-P. Kim, R.S. Ruoff and V.B. Shenoy, *Thermal Transport Across Twin Grain Boundaries in Polycrystalline Graphene from Nonequilibrium Molecular Dynamics Simulations*, Nano Lett., 2011, vol. 11, no. 9, pp. 3917–3921.
- [29] F. Banhart, J. Kotakoski and A.V. Krasheninnikov, *Structural Defects in Graphene*, ACS Nano, 2010, vol.5, no. 1, pp. 26–41.
- [30] L. Liu, M. Qing, Y. Wang and S. Chen, *Defects in Graphene: Generation, Healing, and Their Effects on the Properties of Graphene: A Review*, J. Mater. Sci. Technol., 2015, vol. 31, no. 6, pp. 599–606.
- [31] J. Kotakoski, A. V. Krasheninnikov, U. Kaiser and J.C. Meyer, *From Point Defects in Graphene to Two-Dimensional Amorphous Carbon*, Phys. Rev. Lett., 2011, vol. 106, no. 10, art. 105505.
- [32] K. Kim, Z. Lee, W. Regan, C. Kisielowski, M.F. Crommie and A. Zettl, *Grain Boundary Mapping in Polycrystalline Graphene*, ACS Nano, 2011, vol. 5, no. 3, pp. 2142–2146.
- [33] W.F. Harris, *Disclinations*, Scientific American, 1977, vol. 237, no. 6, pp. 130-145.
- [34] M.A. Rozhkov, A. L. Kolesnikova, I. S. Yasnikov and A. E. Romanov, *Disclination Ensembles in Graphene*, Low Temp. Phys., 2018, vol. 44, no. 9, pp. 918–924.
- [35] A.E. Romanov, M.A. Rozhkov and A.L. Kolesnikova, *Disclinations in Polycrystalline Graphene and Pseudo-Graphenes. Review*, Lett. Mater., 2018, vol. 8, no. 4, pp. 384–400.
- [36] R.H. Baughman, H. Eckhardt and M. Kertesz, *Structure-property Predictions for New Planar Forms of Carbon: Layered Phases Containing sp^2 and sp Atoms*, J. Chem. Phys., 1987, vol. 87, no. 11, pp. 6687–6699.
- [37] A.N. Enyashin and A.L. Ivanovskii, *Graphene Allotropes*, Phys. Stat. Sol. (b), 2011, vol. 248, no. 8, pp. 1879–1883.
- [38] Z. Gong, X. Shi, J. Li, S. Li, C. He, T. Ouyang, C. Zhang, C. Tang and J. Zhong, *Theoretical Prediction of Low-Energy Stone-Wales Graphene with an Intrinsic Type-III Dirac Cone*, Phys. Rev. B, 2020, vol. 101, no. 15, art. 155427.
- [39] H. Terrones, M. Terrones, E. Hernández, N. Grobert, J.-C. Charlier and P.M. Ajayan, *New Metallic Allotropes of Planar and Tubular Carbon*, Phys. Rev. Lett., 2000, vol. 84, no. 8, pp. 1716–1719.
- [40] Z. Wang, X.-F. Zhou, X. Zhang, Q. Zhu, H. Dong, M. Zhao and A.R. Oganov, *Phagraphene: A Low-Energy Graphene Allotrope Composed of 5–6–7 Carbon Rings with Distorted Dirac Cones*, Nano Lett., 2015, vol. 15, no. 9, pp. 6182–6186.
- [41] Z. Zhuo, X. Wu and J. Yang, *Me-graphene: a Graphene Allotrope with near Zero Poisson's Ratio, Sizeable Band Gap, and High Carrier Mobility*, Nanoscale, 2020, vol. 12, no. 37, pp. 19359–19366.
- [42] J. Deb, D. Paul and U. Sarkar, *Pentagraphyne: a New Carbon Allotrope with Superior Electronic and Optical Property*, J. Mater. Chem. C, 2020, vol. 8, no. 45, pp. 16143–16150.
- [43] S. Zhang, J. Zhou, Q. Wang, X. Chen, Y. Kawazoe and P. Jena, *Penta-Graphene: A New Carbon Allotrope*, Proc. Natl. Acad. Sci. U.S.A., 2015, vol. 112, no. 8, pp. 2372–2377.
- [44] M.A. Rozhkov, A.L. Kolesnikova, I.S. Yasnikov and A.E. Romanov, *Disclination Ensembles in Graphene*, Low Temp. Phys., 2018, vol. 44, no. 9, pp. 918–924.
- [45] M.A. Rozhkov, A.L. Kolesnikova, I. Hussainova, M.A. Kaliteevskii, T.S. Orlova, Yu.Yu. Smirnov, I.S. Yasnikov, L.V. Zhigilei, V.E. Bougrov and A.E. Romanov, *Evolution of Dirac Cone in Disclinated Graphene*, Rev. Adv. Mater. Sci., 2018, vol. 57, no. 2, pp. 137-142.
- [46] B. Ram and H. Mizuseki, *Tetrahexcarbon: A Two-dimensional Allotrope of Carbon*, Carbon, 2018, vol. 137, pp. 266–273.
- [47] Q. Xie, L. Wang, J. Li, R. Li and X.-Q. Chen, *General Principles to High-Throughput Constructing Two-Dimensional Carbon Allotropes*, Chin. Phys. B, 2020, vol. 29, no. 3, art. 037306.
- [48] Y. Shen, J. Yu, J. Liu, Y. Guo, Y. Qie and Q. Wang, *PCF-Graphene: A 2D sp^2 -Hybridized Carbon Allotrope with a Direct Band Gap*, J. Phys. Chem. C, 2019, vol. 123, no. 7, pp. 4567–4573.
- [49] S.W. Cranford and M.J. Buehler, *Mechanical Properties of Graphyne*, Carbon, 2011, vol. 49, no. 13, pp. 4111–4121.

- [50] A.L. Kolesnikova, M.A. Rozhkov, I. Hussainova, T.S. Orlova, I.S. Yasnikov, L.V. Zhigilei and A.E. Romanov, *Structure and Energy of Intercrystallite Boundaries in Graphene*, Rev. Adv. Mater. Sci., 2017, vol. 52, no. 1/2, pp. 91-98.
- [51] V.I. Vladimirov and A.E. Romanov, *Disclinations in Crystals* (Nauka, Leningrad, 1986), In Russian.
- [52] A.E. Romanov and V.I. Vladimirov, *Disclinations in Crystalline Solids*, In: Dislocations in Solids, vol. 9, ed. by F.R.N. Nabarro (North-Holland, Amsterdam, 1992), p. 191-402.
- [53] I.S. Yasnikov, A.L. Kolesnikova and A.E. Romanov, *Multi-disclination Configurations in Pentagonal Microcrystals and Two-Dimensional Carbon Structures*, Phys. Sol. State, 2016, vol. 58, no. 6, pp. 1184-1190.
- [54] M.A. Rozhkov, N.D. Abramenko, A.L. Kolesnikova and A.E. Romanov, *Zero Misorientation Interfaces in Graphene*, Lett. Mater., 2020, vol. 10, no. 4s, pp. 551-557.
- [55] W. Kohn and L.J. Sham, *Self-Consistent Equations Including Exchange and Correlation Effects*, Phys. Rev., 1965, vol. 140, no. 4A, pp. A1133-A1138.
- [56] <https://www.vasp.at/>
- [57] <https://www.quantum-espresso.org/>
- [58] J.P. Perdew, K. Burke and M. Ernzerhof, *Generalized Gradient Approximation Made Simple*, Phys. Rev. Lett., 1996, vol. 77, no. 18, pp. 3865-3868.
- [59] G. Gui, J. Li and J. Zhong, *Band Structure Engineering of Graphene by Strain: First-Principles Calculations*, Phys. Rev. B, 2008, vol. 78, no. 7, art. 075435.
- [60] I.V. Lebedeva, A.S. Minkin, A.M. Popov and A.A. Knizhnik, *Elastic Constants of Graphene: Comparison of Empirical Potentials and DFT Calculations*, Physica E: Low Dimens. Syst. Nanostruct., 2019, vol. 108, pp. 326-338.
- [61] B.D. Kong, S. Paul, M.B. Nardelli and K.W. Kim, *First-principles Analysis of Lattice Thermal Conductivity in Monolayer and Bilayer Graphene*, Phys. Rev. B, 2009, vol. 80, no. 3, art. 033406.
- [62] S.J. Stuart, A.B. Tutein and J.A. Harrison, *A Reactive Potential for Hydrocarbons with Intermolecular Interactions*, J. Chem. Phys., 2000, vol. 112, no. 14, pp. 6472-6486.
- [63] J. Tersoff, *Empirical Interatomic Potential for Silicon with Improved Elastic Properties*, Phys. Rev. B, 1988, vol. 38, no. 14, pp. 9902-9905.
- [64] K. Chenoweth, A.C.T. van Duin and W.A. Goddard, *ReaxFF Reactive Force Field for Molecular Dynamics Simulations of Hydrocarbon Oxidation*, J. Phys. Chem. A, 2008, vol. 112, no. 5, pp. 1040-1053.
- [65] <https://lammps.sandia.gov/>
- [66] D. Akinwande, C.J. Brennan, J.S. Bunch, P. Egberts, J.R. Felts, H. Gao, R. Huang, J.-S. Kim, T. Li, Y. Li, K.M. Liechti, N. Lu, H.S. Park, E.J. Reed, P. Wang, B.I. Yakobson, T. Zhang, Y.-W. Zhang, Y. Zhou and Y. Zhu, *A Review on Mechanics and Mechanical Properties of 2D Materials—Graphene and Beyond*, Extreme Mech. Lett., 2017, vol. 13, pp. 42-77.
- [67] S. Winczewski, M.Y. Shaheen and J. Rybicki, *Interatomic Potential Suitable for the Modeling of Penta-Graphene: Molecular Statics/ Molecular Dynamics Studies*, Carbon, 2018, vol. 126, pp. 165-175.
- [68] J. Zhao, N. Wei, Z. Fan, J.-W. Jiang, and T. Rabczuk, *The Mechanical Properties of Three Types of Carbon Allotropes*, Nanotechnology, 2013, vol. 24, no. 9, art. 095702.
- [69] B.G. Kim and H.J. Choi, *Graphyne: Hexagonal Network of Carbon with Versatile Dirac Cones*, Phys. Rev. B, 2012, vol. 86, no. 11, art. 115435.
- [70] R. Majidi, *Density Functional Theory Study on Structural and Mechanical Properties of Graphene, T-graphene, and R-graphyne*, Theor. Chem. Acc., 2017, vol. 136, no. 9, art. 109.
- [71] H. Lu and S.-D. Li, *Two-dimensional Carbon Allotropes from Graphene to Graphyne*, J. Mater. Chem. C, 2013, vol. 1, no. 23, art. 3677.
- [72] X. Li, Q. Wang and P. Jena, *ψ -Graphene: A New Metallic Allotrope of Planar Carbon with Potential Applications as Anode Materials for Lithium-Ion Batteries*, J. Phys. Chem. Lett., 2017, vol. 8, no. 14, pp. 3234-3241.
- [73] W.-J. Yin, Y.-E. Xie, L.-M. Liu, R.-Z. Wang, X.-L. Wei, L. Lau, J.-X. Zhong and Y.-P. Chen, *R-graphyne: a New Two-dimensional Carbon Allotrope with Versatile Dirac-like Point in Nanoribbons*, J. Mat. Chem. A, 2013, vol. 1, no. 17, art. 5341.

- [74] D. Bhattacharya and D. Jana, *Twin T-graphene: a New Semiconducting 2D Carbon Allotrope*, Phys. Chem. Chem. Phys., 2020, vol. 22, no. 18, pp. 10286–10294.
- [75] W. Zhang, C. Chai, Q. Fan, Y. Song and Y. Yang, *PBCF-Graphene: a 2D sp^2 Hybridized Honeycomb Carbon Allotrope with a Direct Band Gap*, ChemNanoMat, 2019, vol. 6, no. 1, pp. 139–147.
- [76] J.-W. Jiang, J. Leng, J. Li, Z. Guo, T. Chang, X. Guo and T. Zhang, *Twin Graphene: A Novel Two-Dimensional Semiconducting Carbon Allotrope*, Carbon, 2017, vol. 118, pp. 370–375.
- [77] Y. Zhang, T.T. Tang, C. Girit, Z. Hao, M.C. Martin, A. Zettl, M.F. Crommie, Y.R. Shen and F. Wang, *Direct Observation of a Widely Tunable Bandgap in Bilayer Graphene*, Nature, 2009, vol. 459, no. 7248, pp. 820–823.
- [78] V. H. Crespi, L. X. Benedict, M. L. Cohen and S. G. Louie, *Prediction of a Pure-Carbon Planar Covalent Metal*, Phys. Rev. B., 1996, vol. 53, no. 20, pp. R13303–R13305.
- [79] C. Kou, Y. Tian, M. Zhang, E. Zurek, X. Qu, X. Wang, K. Yin, Y. Yan, L. Gao, M. Lu and W. Yang, *M-Graphene: a Metastable Two-Dimensional Carbon Allotrope*, 2D Materials, 2020, vol. 7, no. 2, art. 025047.
- [80] Z.G. Fthenakis and N.N. Lathiotakis, *Graphene Allotropes Under Extreme Uniaxial Strain: an Ab Initio Theoretical Study*, PCCP, 2015, vol. 17, no. 25, pp. 16418–16427.
- [81] X.-L. Sheng, H.-J. Cui, F. Ye, Q.-B. Yan, Q.-R. Zheng and G. Su, *Octagraphene as a Versatile Carbon Atomic Sheet for Novel Nanotubes, Unconventional Fullerenes, and Hydrogen Storage*, J. Appl. Phys., 2012, vol. 112, no. 7, art. 074315.
- [82] C.-P. Tang and S.-J. Xiong, *A Graphene Composed of Pentagons And Octagons*, AIP Advances, 2012, vol. 2, no. 4, art. 042147.
- [83] M.P. Molepo, R.E. Mapasha, K.O. Obodo and N. Chetty, *First Principles Calculations of Pentaheptite Graphene and Boronitrene Derivatives*, Comput. Mater. Sci., 2014, vol. 92, pp. 395–400.
- [84] A.I. Podlivaev and L.A. Openov, *Kinetic Stability of Octagraphene*, Phys. Solid State, 2013, vol. 55, no. 12, pp. 2592–2595.
- [85] Q. Gu, D. Xing and J. Sun, *Superconducting Single-Layer T-Graphene and Novel Synthesis Routes*, Chinese Phys. Lett., 2019, vol. 36, no. 9, art. 097401.
- [86] T. Morresi, A. Pedrielli, S.A. Beccara, R. Gabbriellini, N.M. Pugno and S. Taioli, *Structural, Electronic and Mechanical Properties of All- sp^2 Carbon Allotropes with Density Lower Than Graphene*, Carbon, 2019, vol. 159, pp. 512–526.
- [87] L.-C. Xu, R.-Z. Wang, M.-S. Miao, X.-L. Wei, Y.-P. Chen, H. Yan, W.-M. Lau, L.-M. Liu and Y.-M. Ma, *Two Dimensional Dirac Carbon Allotropes From Graphene*, Nanoscale, 2014, vol. 6, no. 2, pp. 1113–1118.
- [88] H. Sun, S. Mukherjee and C. V. Singh, *Mechanical Properties of Monolayer Penta-Graphene and Phagraphene: a First-Principles Study*, PCCP, 2016, vol. 18, no. 38, pp. 26736–26742.
- [89] L.F.C. Pereira, B. Mortazavi, M. Makaremi and T. Rabczuk, *Anisotropic Thermal Conductivity and Mechanical Properties of Phagraphene: a Molecular Dynamics Study*, RSC Advances, 2016, vol. 6, no. 63, pp. 57773–57779.
- [90] M. Deza, P.W. Fowler, M. Shtogrin and K. Vietze, *Pentaheptite Modifications of the Graphite Sheet*, J. Chem. Inf. Comput. Sci., 2000, vol. 40, no. 6, pp. 1325–1332.
- [91] U.H.F. Bunz, Y. Rubin and Y. Tobe, *Polyethynylated Cyclic π -Systems: Scaffoldings for Novel Two And Three-Dimensional Carbon Networks*, Chem. Soc. Rev., 1999, vol. 28, no. 2, pp. 107–119.
- [92] B. Ram and H. Mizuseki, *C568: A New Two-Dimensional sp^2 - sp^3 Hybridized Allotrope of Carbon*, Carbon, 2020, vol. 158, pp. 827–835.
- [93] N. Narita, S. Nagai, S. Suzuki and K. Nakao, *Optimized Geometries and Electronic Structures of Graphyne and its Family*, Phys. Rev. B, 1998, vol. 58, no. 16, pp. 11009–11014.
- [94] B. Zou, J. Shen, P. Yu and J. Zhao, *The Young's Moduli of Three Types of Carbon Allotropes: a Molecular Mechanics Model and a Finite-Element Method*, Proc. Roy. Soc. A, 2016, vol. 472, no. 2186, art. 20150628.
- [95] H. Gao and W. Ren, *Emergence of Type-I and Type-II Dirac Line Nodes in Penta-Octa-Graphene*, Carbon, 2020, vol. 158, pp. 210–215.
- [96] J. Hou, Z. Yin, Y. Zhang and T.C. Chang, *Structure Dependent Elastic Properties of Supergraphene*, Acta Mech.Sinica, 2016, vol. 32, no. 4, pp. 684–689.

- [97] Y. Wang, A.J. Page, Y. Nishimoto, H.J. Qian, K. Morokuma and S. Irle, *Template Effect in the Competition Between Haeckelite and Graphene Growth on Ni(111): Quantum Chemical Molecular Dynamics Simulations*, J. Am. Chem. Soc., 2011, vol. 133, no. 46, pp. 18837–18842.
- [98] M.A. Rozhkov, *Mechanical and Electrical Properties of Graphene Crystals with Disclinations*, PhDThesis, (ITMO University, 2019), In Russian.
- [99] F. Q. Wang, J. Yu, Q. Wang, Y. Kawazoe and P. Jena, *Lattice Thermal Conductivity of Penta-Graphene*, Carbon, 2016, vol. 105, pp. 424–429.
- [100] <https://uspex-team.org/>.

(c) ITMO 2020