

Molecular Dynamics of Thermal Stability of Graphene Nanostructures for Nanoelectronics Devices

Fagbenro AB^{1*}, Sigalo FB², Adekanmbi M³, Onuikpe PC⁴, Emelue HU¹, and Ajana O¹

¹Department of Physics Faculty of Science Alvan Ikoku Federal University of Education Owerri Imo State

²Department of Physics, Faculty of Science Rivers State University, Port Harcourt, Rivers State

³Department Of Physics Faculty of Natural and Applied Science Ignatius Ajuru University of Education Port Harcourt River State

⁴Department of Physics, Abubakar Tafawa Balewa University, Bauchi

*Corresponding author:

Fagbenro AB, Department of Physics Faculty of Science Alvan Ikoku Federal University of Education Owerri Imo State.

ABSTRACT

In this study we investigated the thermal stability of graphene structure (sheet) as a function of temperature using molecular dynamics (MD) simulations with the Tersoff potential. Graphene sheet consisting of 1380 carbon atoms were subjected to temperature range of 4500 K to 5500 K which is meant to simulate extreme thermal conditions where significant structural changes are expected. Four metrics were used to quantify the thermal stability, these are (i) average number of bonds count (ii) the average coordination number, (iii) the fraction of hexagonal rings, and (iv) the average bond length. These metrics are extracted from molecular dynamics trajectories and were analyzed. Results show a progressive decomposition of the graphene lattice, which implies by controlling these structural metrics, graphene can be tailored for specific applications in nanoelectronics, such as high-speed transistors, flexible electronics, sensors, and memory devices.

Keywords: Molecular Dynamics, Graphene, Nanoelectronics, Tersoff Potential.

Received: June 10, 2026;

Accepted: June 17, 2026;

Published: September 04, 2026

Introduction

Graphene is a two-dimensional allotrope of carbon atoms arranged in a hexagonal lattice; it has attracted immense research interest due to its unique electrical, mechanical, and thermal properties. Its nanoscale dimensions and high thermal conductivity make it a promising candidate for applications in nanoelectronics, thermal management, and flexible electronic devices. Heat can be transfer by conduction, convection and radiation process with the heat carrier being electrons, photons, phonons, atoms or molecules [1].

First-principle based approach are very useful in accurately predicting the thermal transport properties of materials and revealing the phonon and electron scattering or propagation mechanism in material and electronic devices [2].

A single layer peeled from graphite reveals graphene, a two-dimensional allotrope consisting of a single atomic layer of carbon atoms arranged in a honeycomb lattice. Since its experimental isolation in 2004, graphene has revolutionised carbon materials research due to its exceptional mechanical strength, high carrier mobility, and thermal conductivity [3]. It is often described as the building block of other carbon allotropes: graphene layers stack to form graphite; they can be rolled into carbon nanotubes or wrapped into fullerenes, highlighting graphene's central role in carbon nanostructures [4].

The ability of these carbon allotropes to exist in such diverse structural forms makes them ideal candidates for molecular dynamics (MD) simulations, which rely on atomistic modelling to explore material properties.

Citation: Fagbenro AB, Sigalo FB, Adekanmbi M, Onuikpe PC, Emelue HU, and Ajana O (2026) Molecular Dynamics of Thermal Stability of Graphene Nanostructures for Nanoelectronics Devices. J All Phy Res Appli 2: 1-6.

Among these allotropes, graphene stands out as a model system for investigating thermal, mechanical, and electronic phenomena at the nanoscale. MD simulations provide a powerful approach to study how graphene behaves under different conditions such as temperature variations, mechanical loading, and chemical doping by tracking atomic interactions over time [5]. In a solid form, the density of graphene is 1g/cm³. Graphene is stable due to its strong covalent planar bonds [4]. It is about 0.34nm thick and composed of carbon atoms that are arranged hexagonally in a honeycomb structure.

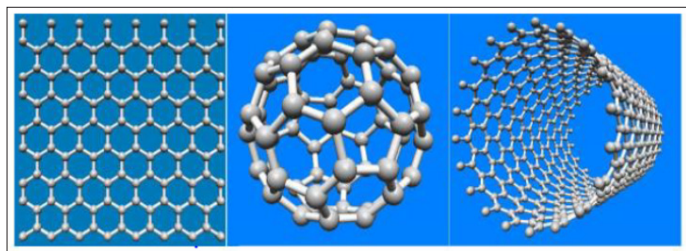


Plate 1: (a) Structure of graphene (b) Fullerenes. (c) Carbon nanotubes. Source: (Nakhate., 2015) [6].

The ability of these carbon allotropes to exist in such diverse structural forms makes them ideal candidates for molecular dynamics (MD) simulations, which rely on atomistic modelling to explore material properties. Among these allotropes, graphene stands out as a model system for investigating thermal, mechanical, and electronic phenomena at the nanoscale. MD simulations provide a powerful approach to study how graphene behaves under different conditions such as temperature variations, mechanical loading, and chemical doping by tracking atomic interactions over time [5]. In a solid form, the density of graphene is 1g/cm³. Graphene is stable due to its strong covalent planar bonds [4]. It is about 0.34nm thick and composed of carbon atoms that are arranged hexagonally in a honeycomb structure.

In recent years, the use of classical MD simulations, particularly with interatomic potentials such as the Tersoff and REBO force fields, has proven to be effective in capturing the essential physical interactions within graphene structures. These models have been instrumental in predicting changes in bond lengths, coordination numbers, phonon dispersion, and thermal conductivity in both pristine and doped graphene sheets [7]. Moreover, advancements in computational resources and parallel processing have enabled longer simulation times and larger system sizes, further enhancing the reliability and applicability of MD methods in materials research.

Literature Review

In research carried out by Zakharchenko et al. on the Melting of graphene [8]. Temperature dependence of the lattice parameter, elastic properties, and heat capacity was calculated by means of atomistic Monte Carlo simulations which is large-scale MD simulations. It was observed that graphene remains structurally intact until about 4900 K, where it eventually undergoes sublimation. He concluded that Graphene does not melt in the traditional sense but undergoes sublimation as the C-C bonds break down under high temperatures.

In a work by Lukas et al. on the topic: Low-temperature Thermal Transport in Moiré Superlattices [9]. He calculates the phonon thermal conductivity of various moiré bilayer systems using a continuum approach and the semiclassical transport theory. He noticed that when the twist angle is close to 0, there is reduction of thermal conductivity in a particular low-temperature regime. The reduction was attributed to a moiré-induced reconstruction of acoustic phonon bands and associated decrease of the group velocity.

In the work carried out by Baladin et al., on the superior thermal conductivity of single-layer graphene [10]. The experimental investigation of thermal conduction in a suspended single-layer graphene was performed with the help of confocal micro-Raman spectroscopy. By using a noncontact optical-based technique, it was discovered that graphene manifests an extraordinarily high room temperature (RT) thermal conductivity of up to $(5.30 \pm 0.48) \times 10^3$ W/mK. The measurements were performed for an individual single-layer graphene suspended over a wide trench in Si/SiO₂ substrate. The extracted thermal conductivity of graphene is larger than conventionally accepted experimental values reported for individual suspended carbon nanotubes (CNTs) and corresponds to the upper bound of the highest values reported for single-wall CNT bundles.

In the work carried out by Galashev and Rakhmanova on the mechanical and thermal stability of graphene and graphene-based materials [11]. Based Molecular Dynamics simulation, the strong plastic deformation of compression in the zigzag and armchair directions of a free-standing graphene sheet was studied. A different behavior of the graphene sheet was revealed when these deformations were present. The compression along the zigzag direction weakens the edges of the sheet parallel to this direction because of the local destruction of the cellular hexagonal structure along the lower and upper edges of the sheet. In the final account, after the implementation of 59 acts of compression through compression stress (ϵ) = 0.0058, the graphene sheet retained its integrity, only a small number of C atoms was lost. The defect cellular hexagonal structure was retained in the H form but along the armchair direction, the graphene sheet was unable to sustain such strong stresses of compression. Compression along the zigzag direction causes carbon C atoms to begin to escape from the sheet in the vertical direction (along the z-axis) already under relative deformations (ϵ) = 0:0235, and upon compression along the armchair direction, at (ϵ) = 0:0266. A further compression of the sheet leads to an increase in the number of atomic displacements in the z direction.

Methodology

Model Construction and Simulation Setup: The thermal stability of graphene nanostructures was investigated using classical Molecular Dynamics (MD) simulations implemented in the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS). A single-layer graphene sheet was constructed with periodic boundary conditions applied along the in-plane directions (x and y axes), while a sufficiently large vacuum region was introduced along the out-of-plane direction (z-axis) to eliminate interactions between periodic images. The initial

atomic configuration was generated based on the hexagonal lattice structure of graphene with an equilibrium carbon-carbon bond length of approximately 1.42 Å.

Prior to thermal analysis, the graphene structure was subjected to energy minimization using the conjugate gradient algorithm to remove residual stresses and obtain a stable equilibrium configuration. This step ensured that the subsequent thermal simulations accurately represented the intrinsic behavior of the material.

Interatomic Potential: The interactions between carbon atoms were described using the Tersoff potential, a many-body empirical potential widely employed for covalently bonded materials. The Tersoff potential accounts for bond-order effects and accurately captures bond formation, bond breaking, and atomic rearrangements under varying thermal conditions. Consequently, it is particularly suitable for investigating the structural evolution and thermal stability of graphene at elevated temperatures.

The total interaction energy of the system is determined by a combination of attractive and repulsive pair interactions modulated by a bond-order term, enabling realistic representation of the atomic-scale behavior of graphene under thermal loading.

Equilibration Procedure: Following energy minimization, the system was equilibrated at room temperature (300 K) using the canonical ensemble (NVT), controlled by the Nosé–Hoover thermostat. The simulations were performed with a time step of 1 fs to ensure numerical stability and accurate integration of atomic trajectories. Equilibration was continued until the temperature and total energy fluctuations reached steady-state conditions, indicating thermal equilibrium.

Thermal Stability Analysis: To evaluate the thermal stability of graphene, the temperature of the system was gradually increased from room temperature to high-temperature regimes relevant to nanoelectronic applications. Simulations were conducted at discrete temperature intervals to monitor the structural response of the graphene lattice under increasing thermal stress. At each temperature, the system was allowed to reach equilibrium before data collection. The thermal stability of the graphene nanostructure was assessed through the analysis of potential energy, atomic displacement, structural ordering, and bond integrity.

Structural Characterization: The evolution of the graphene structure during heating was quantified using several thermodynamic and structural parameters.

Potential Energy Analysis: The variation of potential energy with temperature was monitored to identify changes in the energetic state of the system. A sudden increase in potential energy was considered an indication of structural degradation and the onset of thermal instability.

Mean Square Displacement (MSD): The mobility of carbon atoms was evaluated using the mean square displacement

(MSD). Increasing MSD values with temperature reflect enhanced atomic vibrations and diffusion processes. A sharp rise in MSD was interpreted as evidence of lattice destabilization and loss of structural integrity.

Radial Distribution Function (RDF): The radial distribution function was employed to investigate the degree of atomic ordering within the graphene lattice. Well-defined RDF peaks indicate a highly ordered crystalline structure, whereas peak broadening and intensity reduction signify increasing disorder and thermal-induced structural degradation.

Bond-Length Distribution: The average carbon-carbon bond length was monitored throughout the simulations. Significant deviations from the equilibrium bond length were used as indicators of bond stretching, defect formation, and eventual bond rupture at elevated temperatures.

Visualization and Structural Assessment: Atomic trajectories generated during the simulations were analyzed using visualization software such as OVITO. Structural snapshots obtained at different temperatures were examined to identify lattice distortions, rippling effects, vacancy formation, defect propagation, and possible structural collapse. These visual observations complemented the quantitative analyses obtained from energy and structural calculations.

Determination of Thermal Stability Threshold: The thermal stability threshold of graphene was determined by identifying the temperature at which significant structural deterioration occurred. This threshold was characterized by abrupt changes in potential energy, substantial increases in atomic displacement, loss of crystalline ordering in the RDF profiles, and the emergence of irreversible defects within the graphene lattice. The corresponding temperature was defined as the critical thermal stability temperature, beyond which the graphene nanostructure could no longer maintain its structural integrity for reliable nanoelectronics device operation.

Data Collection

Compute the heat flux $\mathbf{J}(t)$, which is the energy flux through a specific region of the material.

The thermal structural stability κ is then related to the autocorrelation function of the heat flux using the formula:

$$\kappa = \frac{1}{3K_B T^2 V} \int_0^\infty \langle J(0) \cdot J(t) \rangle dt \quad (1)$$

In LAMMPS, we used the `fix ave/correlate` command to collect time-correlation data of the heat flux. A typical calculation in LAMMPS involves running a simulation over a long time to gather enough data for the autocorrelation function.

Results and Discussion

Result of structural stability of graphene: Bond count, hexagonal fraction, bond length and coordination number

Result of structural stability of graphene

Temp (k)	Bond Count	Hexagonal Fraction	Bond length(Å)	Avg Coordination Number
4500	1868.0	0.986591304347826	1.44907460948891	2.99321159420289
4600	1733.0	0.926298550724637	1.46487491225258	2.96133333333333
4700	1588.0	0.785582608695652	1.46925217300921	2.87853913043478
4800	1437.0	0.584544927536231	1.46891343705322	2.73559420289855
4900	1311.0	0.394081159420289	1.46976160471020	2.55557101449275
5000	1200.0	0.252936231884058	1.47254598198489	2.36693333333333
5100	1107.0	0.161886956521739	1.47213031192069	2.19609565217391
5200	1038.0	0.111997101449275	1.47409806362021	2.06034492753623
5300	986.0	0.082156521739130	1.47539695805808	1.95577391304347
5400	953.0	0.066669565217391	1.47668403723355	1.89037101449275
5500	943.0	0.062072463768115	1.47903453108686	1.86469855072467

The result of structural thermal stability was assessed using the following metrics: Bond count, hexagonal fraction, bond length and coordination number

The Result of the Bond Count: The "Bond Count vs. Temperature" plot (Figure 1) shows a steady decrease in the average number of bonds from approximately 1900 at 4500K to 900 at 5500K. In a pristine graphene sheet with 1380 atoms. The result indicated a rapid thermal disruption of atomic bonding as kinetic energy overcomes the cohesive forces in the lattice of graphene structure. At temperature of 5000K – 5500K the bond count decreases at a slower rate this suggested that the majority of easily breakable bonds have already dissociated and the remaining bonds are more thermally stable or represent a disordered state approaching thermal decomposition. The result for the bond count is within the results obtained by Zakharchenko et al. and Xu et al., that showed increased thermal energy leads to bond weakening, bond angle distortions, and eventual lattice breakdown in carbon-based nanomaterials [8,12].

The result of the Hexagonal Fraction: The hexagonal ring fraction vs. temperature plot (Figure 2) provides a direct measure of the graphene lattice's structural integrity, as the hexagonal rings are the fundamental building blocks of the honeycomb lattice. The result shows a fraction decreases from 1.0 at 4500K to 0.1 at 5500K. High fraction occurred at a lower Temperatures between 4500k – 4700K. The hexagonal ring fraction is close to 1.0, indicated that nearly all the carbon atoms are part of a perfect hexagonal structures, just as a typical pristine graphene. This shows the structural integrity of the graphene sheet at lower temperatures. As the temperature increases (4700K to 5000K) the hexagonal fraction drops rapidly, indicating that thermal agitation is breaking the hexagonal symmetry introducing vacancies and defects a sign of structural disorder. As the temperature increases beyond 5100K only a very small fraction of the original hexagonal lattice remains intact. The trend of the result corresponds to the research reported by Los et al. indicating that elevated temperature converted hexagonal rings into defective non-hexagonal polygons, destabilizing the lattice [13].

The Result of the Bond Length: The bond length vs. temperature plot (Figure 3) shows a slight increase in the average bond length from 1.450 Å at 4500K to 1.480 Å at 5500K. The bond length rises from 1.449 Å to 1.469 Å. This is due to thermal expansion which is higher atomic vibrations at elevated temperatures push atoms slightly further apart. There is Fluctuations within (4700k & 5100K) due to Minor oscillations are observed in bond length due to structural rearrangements, defect formations, or the onset of lattice distortion. As the temperare increases beyond 5100 the bond length rises more consistently, approaching ~1.479 Å at 5500 K. This suggests a more disordered or weakened structure, with bonds stretched near or beyond their stable limits, potentially indicating the precursor to bond rupture or material degradation. The result corresponds to the work of Zakharchenko et al. which shows at high temperatures, graphene's in-plane thermal expansion leads to bond length increases, followed by bond instability and breakage beyond a certain thermal threshold [8].

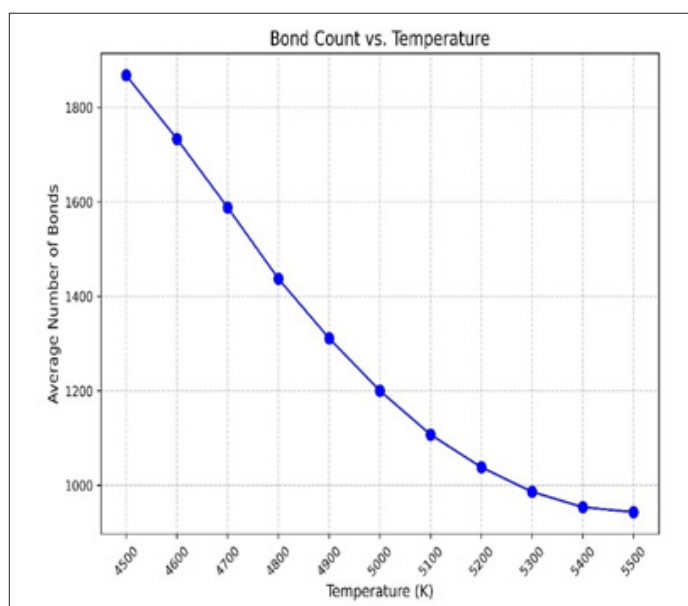


Figure 1: Bond Count against Temperature (k)

The Result of the Coordination Number: The "coordination number vs. temperature" plot (Figure 4) complements the bond count data, showing a decrease in the average coordination number from 3.0 at 4500K to 1.3 at 5500K. The coordination number, defined as $C=N2B$, directly reflects the bond count. At 4500K, the coordination number of 3.0 aligns with the expected value for a pristine graphene sheet (theoretical value 2.92 due to edge effects), confirming that the lattice remains largely intact. The slight discrepancy between the theoretical bond count (2016 $\rightarrow C \approx 2.92$) and the observed value (1900 $\rightarrow C \approx 2.75$) at 4500 K is attributed to thermal defects, consistent with the bond count analysis. The result corresponds to Zakharchenko et al. indicating that Molecular dynamics simulations and neutron scattering experiments have shown that coordination number decreases with temperature in systems like metallic glasses and ionic [8].

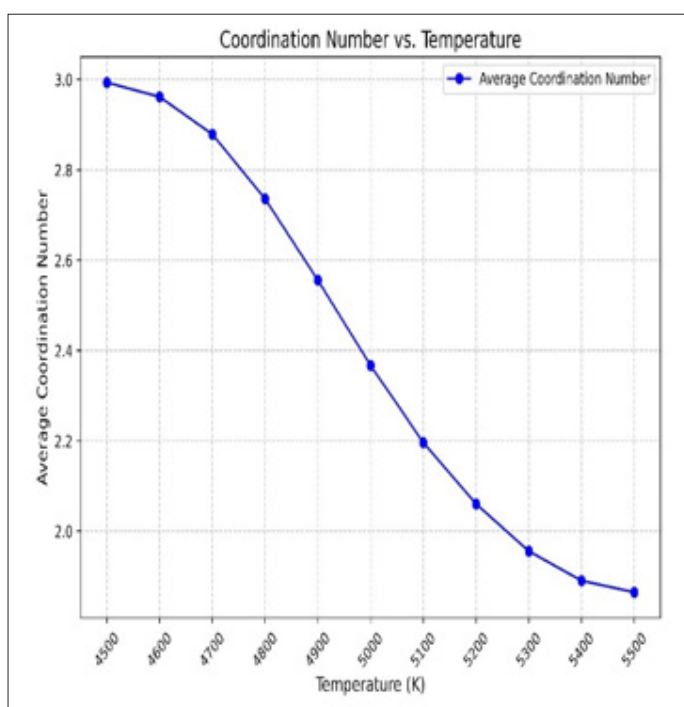


Figure 2: Hexagonal Ring Fraction against Temperature (k)

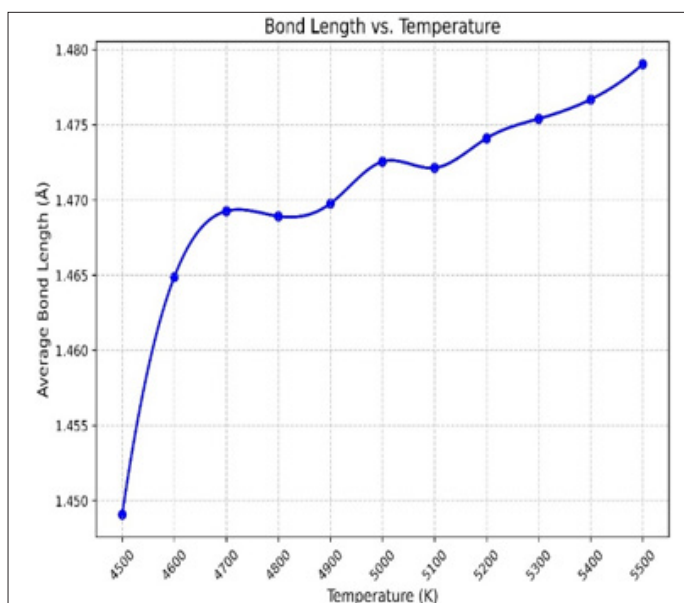


Figure 3: Bond length against Temperature (k)

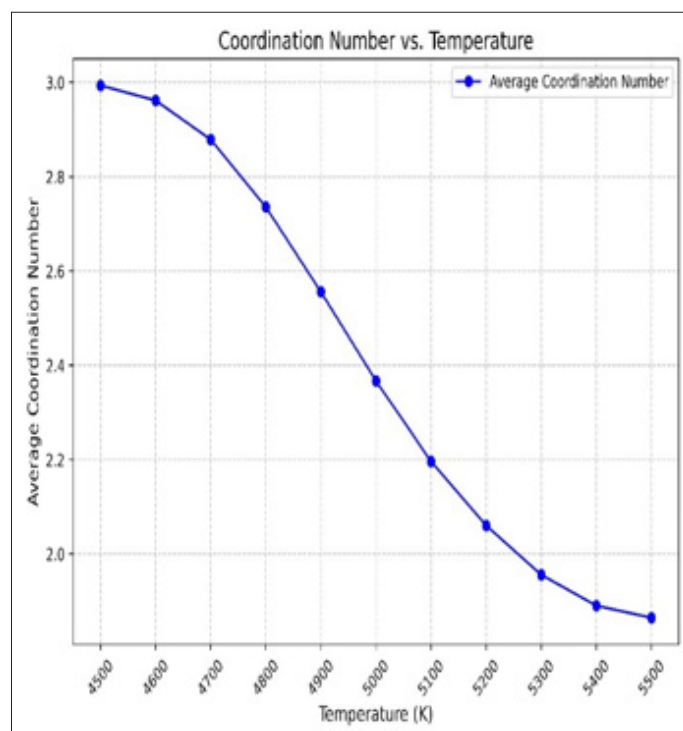


Figure 4: Coordination Number against Temperature (k)

Conclusion

From the detailed simulations and analyses, it can be concluded that thermal transport in graphene is highly sensitive to both temperature and atomic-scale modifications such as doping. As temperature rises, the degradation of the hexagonal framework and the increase in bond length compromise the material's thermal conductivity. While pristine graphene demonstrates excellent thermal stability up to a point, it begins to deteriorate structurally beyond 5100K.

Recommendation

Based on the outcomes of this study focused on elevated temperatures is crucial to simulate thermal transport at more practical operational ranges (500K to 2000K), which are more relevant for device-level applications. Use of Advanced Force Fields; Incorporating more reactive potentials such as ReaxFF in future simulations can be employed in capturing dynamic bond breaking and chemical reactivity under extreme conditions.

References

1. Rani S, Kumar S (2017) Thermal properties of graphene and graphene-based nanostructures for electronic applications: A review. *Journal of Nanoscience and Nanotechnology* 17: 2873–2891.
2. Tengfei M, Pranay C, Xixi G, Lei C, Yan W, et al. (2020) First principles modeling of thermal transport in materials: Achievements, opportunities, and challenges. *International Journal of Thermophysics* 41: 9.
3. Novoselov KS, Geim AK, Morozov SV, Jiang D, Zhang Y, et al. (2004) Electric field effect in atomically thin carbon films. *Science* 306: 666–669.

-
4. Geim AK, Novoselov KS (2007) The rise of graphene. *Nature Materials* 6: 183–191.
 5. Falkovsky LA (2008) Optical properties of graphene. *Journal of Physics: Conference Series* 129: 012004.
 6. Nakhate VV (2015) Thermal properties of graphene (Master's thesis).
 7. Kinaci A, Haskins JB, Sevik C, Çağın T (2012) Thermal conductivity of BN-C nanostructures. *Physical Review B* 86: 115410.
 8. Zakharchenko KV, Los JH, Katsnelson MI, Fasolino A (2009) Melting of graphene: From two to one dimension. *Physical Review Letters* 102: 046808.
 9. Lukas PA Krisna, Takuto Kawakami, Mikito Koshino (2025) Low-temperature Thermal Transport in Moiré Superlattices. *Journal of the Physical Society of Japan* 94.
 10. Balandin AA, Ghosh S, Bao W, Calizo I, Teweldebrhan D, et al. (2008) Superior thermal conductivity of single-layer graphene. *Nano Letters* 8: 902–907.
 11. Galashev AE, Rakhmanova OR (2014) Mechanical and thermal stability of graphene and graphene-based materials. *Physics-Uspekhi* 57: 970–989.
 12. Xu X, Pereira LFC, Wang Y, Wu J, Zhang K, et al. (2014) Length-dependent thermal conductivity in suspended single-layer graphene. *Nature Communications* 5: 3689.
 13. Los JH, Ghiringhelli LM, Meijer EJ, Fasolino A (2005) Improved long-range reactive bond-order potential for carbon: Application to carbon nanotubes and fullerenes. *Physical Review B* 72: 214102.