

Communication



Low and Anisotropic Tensile Strength and Thermal Conductivity in the Single-Layer Fullerene Network Predicted by Machine-Learning Interatomic Potentials

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Abstract: In the latest ground-breaking experimental advancement (*Nature* (2022), 606, 507), zerodimensional fullerenes (C_{60}) have been covalently bonded to form single-layer two-dimensional (2D) fullerene network, namely quasi-hexagonal-phase fullerene (qHPC₆₀). Motivated by the aforementioned accomplishment, in this communication, for the first time, we explore the phononic and mechanical properties of the qHPC₆₀ monolayer, employing state-of-the-art machine-learning interatomic potentials. By employing an efficient passive-training methodology, the thermal and mechanical properties were examined with an ab-initio level of accuracy using the classical molecular dynamics simulations. Predicted phonon dispersion confirmed the desirable dynamical stability of the qHPC₆₀ monolayer. Room temperature lattice thermal conductivity is predicted to be ultralow and around 2.9 (5.7) W/m·K along the x(y) directions, which are by three orders of magnitude lower than that of the graphene. Close to the ground state and at room temperature, the ultimate tensile strength of the qHPC₆₀ monolayer along the x(y) directions is predicted to be 7.0 (8.8) and 3.3 (4.2) GPa, respectively, occurring at corresponding strains of around 0.07 and 0.029, respectively. The presented computationally accelerated first-principles results confirm highly anisotropic and remarkably low tensile strength and phononic thermal conductivity of the qHPC₆₀ fullerene network nanosheets.

Keywords: fullerene network; machine learning; mechanical; thermal conductivity

1. Introduction

Carbon-based two-dimensional (2D) nanomaterials, such as graphene [1–3], are known to exhibit exceptional physical properties, including outstandingly high mechanical [4] and phononic transport [5,6], owing to strong covalent bonding and light-weight atomic lattices. Carbon atoms because of their flexible nature in 2D form can show diverse lattice, such as completely flat graphene, phagraphene [7] and biphenylene [8], or more complex buckled structures, such as fluorinated diamane [9] and pentagraphene [10]. Interestingly, while graphene and phagraphene [7] monolayers are zero-gap semimetals, fluorinated diamane is an insulator [11]. Moreover, despite close energetic stability, the tensile strength and electronic nature of the graphene and phagraphene monolayers, the latter because of non-hexagonal carbon rings, interestingly shows an order of magnitude-suppressed thermal conductivity than graphene [12,13]. It is therefore clear than creating connections between the atomic lattice and resulting physical properties of 2D carbon-based structures is very advantageous for practical employment in nanodevices.

In the latest exciting advancement in the field of 2D materials, most recently by forming carbon–carbon bonds between 0D cages of C_{60} fullerenes, a new sp²–sp³-hybridized full-carbon 2D lattice, single-layer quasi-hexagonal-phase fullerene (qHPC₆₀) has been successfully fabricated by Hou and coworkers [14]. According to the experimental and



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theoretical calculations [14], the single-layer $qHPC_{60}$ is found to be a semiconductor. In order to enhance the understanding of the $qHPC_{60}$ monolayer physical properties, in this communication for the first time, we utilize accurate machine-learning interatomic potentials (MLIPs) to explore the dynamical stability, lattice thermal conductivity, mechanical and failure behavior of this newly synthesized carbon lattice [15–18]. The presented first-principles results provide a unique vision concerning the critical thermo-mechanical properties of the sp^2-sp^3 -hybridized $qHPC_{60}$ nanosheets, which can serve as a valuable guide for future studies on this novel 2D network and any prospective theoretical studies on other 2D lattices.

2. Computational Methods

DFT calculations in this communication were performed using the Vienna Ab-initio Simulation Package [19,20] on the basis of the generalized gradient approximation (GGA) and Perdew-Burke-Ernzerhof (PBE) functional, along with Grimme's DFT-D3 [21] and van der Waal's (vdW) dispersion correction. The plane-wave and self-consistent loop energy cutoff values were set to 500 eV and 10^{-5} eV, respectively. The geometry-optimized lattice was obtained using the conjugate gradient algorithm until Hellman-Feynman forces drop below 0.01 eV/Å [22]. The simulation box size along the out-of-plane direction was set to 22 Å, to elude interaction between them in the three-dimensional periodic systems. In this work, we passively fitted moment tensor potentials (MTPs) [23] to investigate the thermal and mechanical properties at finite temperatures, utilizing the MLIP package [24] and using the same approach employed in our recent works [25,26]. The required datasets for the fitting of MTPs were prepared by conducting ab-initio molecular dynamics (AIMD) simulations within the PBE/GGA and DFT-D3 methods using the VASP package over the unitcell with 120 atoms, time step of 1 fs and 2 \times 2 \times 1 K-point grid. AIMD calculations were conducted for strain-free and -5%, +5%, +10% and +15% biaxially strained samples, in which the systems were heated from 300 to 200 K during 300 time steps. The complete AIMD trajectories were next subsampled, and around 500 configurations were used to train a preliminary MTP. The accuracy of the fitted MTP was then examined over the complete dataset, and configurations with worst extrapolation grades [27] were defined and incorporated to the original dataset. The final MTP with enhanced accuracy and stability was then passively fitted using the improved training dataset. Phonon dispersion relations were obtained using the fitted MTPs over $3 \times 3 \times 1$ supercells and employing the PHONOPY code, as explained in our previous study [28]. Thermal and mechanical properties, on the basis of fitted MTPs, were finally evaluated using the classical molecular dynamics (CMD) simulations, employing the LAMMPS [29] package with a time step of 0.5 fs. Non-equilibrium molecular dynamics (NEMD) simulations were conducted to evaluate the length-dependent lattice thermal transport, using the same approach as that employed in our previous studies [25,30]. Mechanical properties were investigated by employing the quasi-static uniaxial tensile simulations, as explained in our recent studies [25,26,31], with high accuracy, as confirmed by comparing with DFT calculations.

3. Results and Discussion

First, we discuss the atomic and structural features of the energy-minimized qHPC₆₀ monolayer acquired by the DFT simulations, as shown in Figure 1a. The lattice constants of the qHPC₆₀ monolayer along the x(y) directions are predicted to be 15.89 (9.16) Å, respectively, which show excellent agreements with corresponding experimentally measured values of 16.0 (9.17) Å [14]. The in-plane bonding network of the qHPC₆₀ monolayer is clearly anisotropic, in which two individual C₆₀ fullerenes are connected by single titled carbon–carbon bonds along the elongated direction of x. On the other side, two carbon–carbon bonds are oriented exactly along the y direction, directly connecting two separate fullerene cages. The parallel orientation of connecting bonds along the load transfer and the involvement of twice more bonds between two neighboring fullerenes, intuitively suggest stronger mechanical and phonon transport along the y direction. In Figure 1b, the electron

localization function (ELF) [32], with an isosurface value of 0.8, is also illustrated. Large ELF values over 0.8 in the center of bonds, as expected, indicating the formation of strong covalent interactions throughout this novel sp^2-sp^3 -hybridized 2D carbon allotrope. In Figure 1c the phonon dispersion relation of the qHPC₆₀ monolayer on the basis of a trained MTP is depicted. As one of the signatures of 2D materials, this monolayer shows three acoustic phonon modes, initiating from the Γ point. As it can be seen, none of the acoustic and optical modes exhibit imaginary frequencies, confirming the dynamical stability of this novel full-carbon 2D lattice. In the data availability section, we included the energy minimized lattice, along with ELF data and the trained MTP as well.



Figure 1. (a) Top and side views of the $qHPC_{60}$ monolayer. (b) Electron localization function (ELF) with an isosurface value of 0.8, plotted using the VESTA package [33]. MTP-based predicted (c) phonon dispersion relation and (d) phonon group velocity (*GV*) of the $qHPC_{60}$ monolayer.

As shown in Figure 1c inset, the two in-plane acoustic modes of the qHPC₆₀ monolayer appear with linear dispersions, whereas the out-of-plane (ZA) counterpart shows quadratic dispersions from the Γ point, in consistency with other famous 2D lattices, such as graphene and h-BN [28]. For optical modes with frequencies larger than 10 THz, it is noticeable that they show relatively flat dispersions, which confirm their low group velocities, consistent with results shown in Figure 1d. In addition, remarkable band crossing is conspicuous throughout the entire frequency range for both in-plane acoustic and optical modes, revealing high scattering and short phonon lifetime along these heat carriers. The combination of low phonon group velocity and high scattering rates suggest remarkably low lattice thermal conductivity along this novel sp²-sp³-hybridized 2D carbon allotrope. As it is also observable from the Figure 1c inset, the out-of-plane ZA is the only phonon mode convincingly free of intersection with other vibrations, which suggests lower scattering rates. In consistency with the lattice thermal transport of graphene [34], BC₆N [30] and BC_2N [35] monolayers, one can also conclude the considerable contribution of ZA phonon mode in the heat transport of the $qHPC_{60}$ monolayer. In accordance with our earlier analysis of structural features, the ZA acoustic mode dispersion is almost two times wider along the Γ -Y path that the Γ -X counterpart, which reveals considerably higher phonon group velocity along the *y* direction. To evaluate the lattice thermal conductivity, we have conducted NEMD simulations. Since in the NEMD simulations of heat conduction, the atoms at the two ends are fixed, the contribution of long wavelength phonons become restricted and thus the effects of length on the lattice thermal conductivity are ought to be examined. In Figure 2, the NEMD results for the length and direction effect on the lattice thermal conductivity of the $qHPC_{60}$ monolayer at room temperature are plotted, assuming a fixed thickness of 12.2 Å, according to that measured experimentally with atomic force microscopy [14]. As it is clear for the NEMD results along the *x* direction, the room temperature lattice thermal conductivity converges to 2.9 ± 0.3 W/m·K for the systems longer than 40 nm. Along the *y* direction, an increasing trend is, however, observable. As a well-established approach, based on the NEMD predictions for the samples with finite lengths of *L*, κ_L , the diffusive phononic thermal conductivity, κ_∞ , can be estimated via [36]:

$$\frac{1}{\kappa_L} = \frac{1}{\kappa_\infty} \left(1 + \frac{\Lambda}{L} \right) \tag{1}$$



Figure 2. MTP-based NEMD results for the length and direction effect on the room temperature phononic thermal conductivity of the qHPC₆₀ monolayer. Continuous line is the fitted function according to Equation (1) to extrapolate the diffusive lattice thermal conductivity (κ_{∞}).

Using the aforementioned relation, the room temperature diffusive lattice thermal conductivity of the qHPC₆₀ monolayer along the *y* direction is predicted to be 5.7 ± 0.5 W/m·K (find the fitted line in Figure 2, which is almost twice of that along the *x* direction). As it is clear, this novel sp²–sp³-hybridized 2D carbon allotrope shows ultralow, by three orders of magnitude lower thermal conductivity than graphene [34], stemmed from high phonon scattering rates and low phonon group velocities. The combination of the semiconducting character with ultralow lattice thermal conductivity might be promising for the thermoelectric energy conversion, which requires a separate study.

Last but not the least, we investigate the anisotropic mechanical response of the $qHPC_{60}$ monolayer by the MTP-based model, using systems with around 1000 atoms. As confirmed in our previous work [25,26,30,31,35], the MTP-based molecular dynamics simulations conducted at 1 K can closely reproduce the ground state DFT results. In Figure 3, the predicted direction-dependent uniaxial stress–strain responses of the $qHPC_{60}$ monolayer

by the MTP-based model at 1 and 300 K are compared. In these results, real volumes of the deformed lattices are considered, assuming a fixed thickness of 12.2 Å [14] during the deformation. Close to the ground state (1 K), the ultimate tensile strength of the $qHPC_{60}$ monolayer along the x(y) directions are predicted to be 7.0 (8.8) GPa. Interestingly, for the both loading directions, the failure occurs at a strain level of 0.07. At room temperature, the ultimate tensile strength of this novel sp^2-sp^3 -hybridized 2D carbon allotrope drop by around 51%, as compared with 1 K, to values of 3.3 (4.2) GPa along the x(y) directions, occurring at a failure strain of around 0.029. In comparison with graphene at 300 K, the ultimate tensile strength of the $qHPC_{60}$ monolayer is more than 20-fold lower [31]. The estimated reduction of around 51% in tensile strengths of the qHPC₆₀ monolayer from 1 to 300 K, is noticeably higher than that observed in other carbon-based 2D materials [25,26,30,31,35]. Our findings not only reveal considerably low and anisotropic tensile strength along this novel sp²-sp³-hybridized 2D carbon allotrope but also reveal anomalous suppression of the tensile strength at high temperatures. As expected, results shown in Figure 3c,d confirm the failure initiation by the breakages of the connecting carbon–carbon bonds. Interestingly, during the failure progress for both the loading directions, several of four-membered connecting carbon rings throughout the monolayer are found to disintegrate and form larger chains. As it is clear, the failure in this novel full-carbon 2D system occurs at low strain levels, which can be an indication of a highly brittle mechanical behavior.



Figure 3. Predicted uniaxial stress–strain responses of the qHPC₆₀ monolayer by MTP-based molecular dynamics simulations carried out at 1 and 300 K along (**a**) x and (**b**) y directions. Close-up view for the failure mechanism for the uniaxial loading along (**c**) x and (**d**) y directions plotted using the OVITO package [37] (for the related videos refer to the data availability).

4. Concluding Remarks

Motivated by the latest experimental advance [14] in the synthesis of covalently bonded single-layer fullerene network, or so called qHPC₆₀ monolayers, as the first study in this communication, we employed moment tensor potentials to examine the dynamical stability and evaluate the complex orientation-dependent mechanical response and lattice thermal transport of this novel sp²–sp³-hybridized 2D carbon allotrope. We found that none of the acoustic and optical modes in this system exhibit imaginary frequencies, confirming its desirable dynamical stability. Room temperature lattice thermal conductivity of the qHPC₆₀ monolayer on the basis of non-equilibrium molecular dynamics (NEMD) simulations were predicted to be ultralow and around 2.9 (5.7) W/m·K along the x(y)directions, which are by three orders of magnitude lower than that of the graphene. Close to the ground state and at 300 K, the ultimate tensile strength of the qHPC₆₀ monolayer along the x(y) directions were predicted to be 7.0 (8.8) and 3.3 (4.2) GPa, respectively, occurring at corresponding low strains of around 0.07 and 0.029, respectively. The failure was found to be highly brittle and was initiated by the breakages of the connecting carbon– carbon bonds between fullerene cages. The estimated reduction in the tensile strengths of the qHPC₆₀ monolayer from 1 and 300 K was found to be anomalous and considerably higher than that previously predicted for other carbon-based 2D materials. The presented first-principles results confirm highly anisotropic and remarkably low tensile strength and thermal conductivity of the qHPC₆₀ fullerene network nanosheets.

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