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Molecular Dynamics Analysis of Virus-Induced Vibrational Changes in Single-layer Graphene

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Summary:
In the past serval years, the COVID-19 pandemic has significantly impacted people's lives, raising concerns about how to effectively mitigate pandemic-related panic. Early detection of airborne viruses could serve as an important means of triggering timely alarms and preventing further spread. Therefore, the development of highly sensitive virus detection technologies is essential. In this work, a novel concept for virus detection using single-layer graphene (SLG) is proposed. The influence of virus attachment on the vibrational behavior of SLG was investigated through molecular dynamics (MD) simulations.

Keywords: single-layer graphene, molecular dynamics simulation, vibrational analysis, mass sensing, virus detection

Background, Motivation an Objective

The COVID-19 pandemic has drastically transformed human life across the globe over the past several years. Although its direct impact has largely diminished, the challenge of preventing future large-scale epidemics remains a pressing concern. One promising strategy is to detect airborne viruses in real time and integrate the information with Internet of Things (IoT) systems, enabling early warnings and helping people avoid contaminated environments. Therefore, the development of rapid and reliable airborne virus detection technologies has become critical [1]. Conventional virus detection methods, such as polymerase chain reaction (PCR), although accurate, are time-consuming, require specialized equipment, and depend heavily on professional expertise. More importantly, traditional PCR methods do not provide real-time data, making them unsuitable for continuous, on-site virus monitoring. This highlights the urgent need for novel, real-time virus detection approaches. In recent years, the emergence of two-dimensional (2D) materials—materials composed of only one or a few atomic layers—has opened up new possibilities in sensing technologies due to their unique physical and chemical properties. Among them, SLG has attracted particular attention [2]. SLG is a one-atom-thick sheet of carbon atoms arranged in a hexagonal lattice, renowned for its exceptional mechanical strength, high electrical and thermal conductivity, and distinctive quantum behaviors. These properties make it highly sensitive to external perturbation, including mass changes caused by adsorbed particles.

Recent studies have demonstrated the potential of SLG in mass sensing applications. For instance, M. Mirakhorya et al. [3] employed MD simulations to investigate the vibrational characteristics of triangular graphene sheets with various geometries, showing that equilateral configurations exhibit the highest resonance frequencies. Similarly, S. Ahmad Fazelzadeh et al. [4] proposed a novel vibration-based mass sensing model for orthotropic SLG with multiple attached nanoparticles, emphasizing the influence of temperature variation, nanoparticle mass and location, and nonlocal effects on the sensor's vibrational response. Given that viruses typically have masses on the order of several attograms, even a single virus adsorbed on an SLG surface may cause detectable shifts in its vibrational behavior. This suggests a new opportunity for highly sensitive virus detection based on monitoring the vibrational response of graphene.

In this work, we propose a novel virus detection technique that utilizes the change in vibrational characteristics of SLG before and after virus attachment. MD simulations were conducted to analyze these vibrational differences, with a focus on the effect of COVID-19 virus attachment on the graphene's dynamic behavior.

Description of the Method

MD simulations were conducted using LAMMPS to investigate the vibrational behavior of SLG before and after the adsorption of the SARS-CoV-

2 main protease [5]. For the initial vibration analysis, a pristine graphene sheet was constructed with its edge atoms fixed to simulate a clamped boundary condition. A pulsed force was applied to the sheet to excite vibrations, and the atomic trajectories were recorded to extract vibrational modes and frequencies (see in Fig. 1).

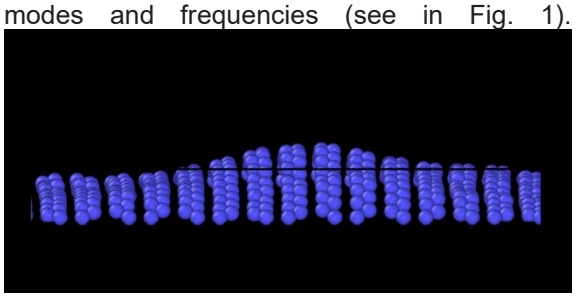

Fig. 1 Schematic of the vibration of SLG.

Prior to the adsorption simulations, the SARS-CoV-2 main protease was coarse-grained to reduce computational complexity while preserving its essential mass distribution and structural integrity. Coarse-graining allows for efficient simulation of large biomolecules, enabling longer simulation times and larger system sizes without significantly compromising the accuracy of mechanical interactions.

Subsequently, the coarse-grained protease was positioned on the central region of the graphene surface. The same fixed boundary conditions were applied, and vibrational excitation was introduced as before. The trajectories of graphene atoms were analyzed to assess changes in vibrational behavior caused by virus adsorption.

Results

The MD simulations showed clear differences in the vibrational behavior of SLG before and after the adsorption of the SARS-CoV-2 main protease. The model used for the simulation is illustrated in Fig. 2. In the pristine state, the graphene sheet exhibited distinct and stable vibrational modes. After virus adsorption, the overall vibrational response changed, with shifts observed in the natural frequencies and slight modifications in the vibration patterns. These changes suggest that the mass and interaction of the adsorbed virus significantly affect the dynamic characteristics of the graphene sheet. The results indicate that monitoring variations in vibrational behavior could serve as an effective approach for detecting the presence of virus particles on graphene surfaces.

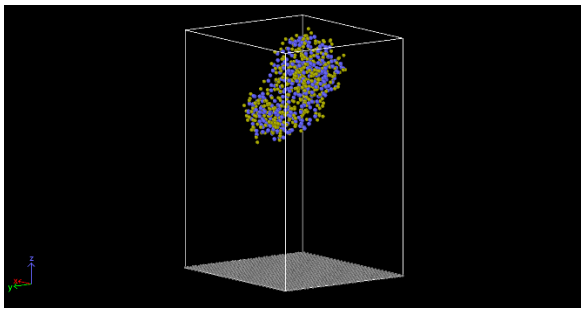

Fig. 2 Model of the SLG and coarse-grained protease.

Conclusion

This study employed MD simulations to investigate the vibrational behavior of SLG before and after virus adsorption. The results showed that virus attachment leads to changes in vibrational behavious, demonstrating the potential of MD-based methods for developing real-time, ultra-sensitive virus detection systems.

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