

# STATEMENT OF PURPOSE

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Like any other geeks, I have strong enthusiasm in gadgets and electronics. Specifically, I care a lot about their performance of heat dissipation because effective thermal management is becoming increasingly important for high-power electronics and portable devices. Phonon plays a key role in determining the thermal properties of semi-conductors and I want to learn related theories, methods and tools systematically to obtain an in-depth understanding of its mechanism as well as effective ways to manage/manipulate phonons in nanoscale during my PhD studies.

I have an excellent academic record, especially in the course of heat transfer and thermodynamics. But most importantly, I am highly-motivated in conducting independent scientific research on nanoscale thermal transport. As a research assistant in Nano Heat Group, my research focuses on reduction of thermal conductivity of graphene for its potential thermoelectric application. Using the fortran code I wrote, I calculated the suspended graphene's thermal conductivity by non-equilibrium molecular dynamics and compared my results with previous work by others to make sure my program is faultless. Afterwards, I changed the structure of the graphene into folded one and took the long-range atom-atom/atom-substrate interaction into consideration. With relatively large size parameter and period boundary condition, the converged outcomes indicate the thermal conductivity of bulk folded graphene. And my results clearly show that thermal conductivity decreases significantly with not only increasing number of folds but stronger substrate effect, which is due to the enhanced phonon scattering. This research provides efficient ways of decreasing thermal conductivity of bulk graphene to increase its figure of merit. And the process of programming, testing, calculating and modifying is just like playing games, challenging but interesting. I enjoy seeing ideas in mind be implemented through programming and simulation. I am confident that both my comprehension of mechanism of nanoscale thermal transport and programming skills were largely improved.

Not limited to research on the relationship between the thermal conductivity and the structure, I also actively collaborate with our group member, Dr. Meng An. The coupling between vibration modes on different directions in graphene has already been studied by others, what we do is to investigate the connection between the length and coupling. Through discussion and exchanging feedback with each other, I learned how to collaborate to overcome adversities together.

Admittedly, I met series of challenges in my simulation research, e.g., programming errors, the limited computing resource, but the genuine interest in nanoscale heat transfer and numerical modeling drive me forward. From these numerical studies, I acquired solid skills and rigorous attitude. Through attending group meeting every week, I catch up with the minds of pioneers. These valuable experiences will greatly contribute to my further study as a graduate student in Virginia Tech.

I always believe that expertise and specialty is the key factor if someone want to contribute to the commonwealth of society, which usually requires years of continuous efforts. Thus I will definitely keep pursuing my academic career in research on heat transfer in nanoscale after my graduation. As the energy shortage became more and more serious, innovative nanostructured materials have attracted attention from researchers and engineers all around the world for their extraordinary performance in energy capture, energy conversion and energy storage, which may possibly become a key to solve the crisis. So many interesting phenomena were newly discovered, e.g. the promising thermoelectric application of  $\text{MoS}_2$  or phosphorene and there are still so many more to be explored. I am so proud of choosing a meaningful path.

Virginia Tech is known for its advanced interdisciplinary studies, especially for research on nanostructured system for energy harvesting and conversion. Some of the faculty are doing remarkable research on fundamental mechanism of thermal transport than deeply intrigues me. I can learn their methods and thoughts them as well as the correct attitude towards science and research through life-long time. I'm looking forward to becoming a distinguished scholar in the future and Virginia Tech seems like a perfect starting point for me.

