AB INITIO MOLECULAR DYNAMICS STUDY OF NANOSCALE HEAT TRANSFER AND ENERGY CONVERSION

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ABSTRACT

In this thesis, ab initio molecular dynamics simulation based on a plane wave/pseudopotential implementation of density functional theory was adopted to investigate nanoscale heat transfer and energy conversions for semiconductors.

The first one investigates the heat conduction process occurring in Si/Ge superlattices at selected stages from the initial point of nonzero temperature gradient to the final state of thermal equilibrium. The second one studies the thermal energy transportation phenomena spanning from heat conduction of thermal radiation with the modeling of variable gap distances in different thin layer systems. The third one presents an ab initio molecular dynamics study of femtosecond laser processing of germanium

As the first work of studying the nanoscale energy transport spanning from heat conduction to thermal radiation and the femtosecond laser material interaction in mechanical engineering, the simulation results highlight the promising application of the first-principles molecular dynamics in thermal engineering. We believe our results and the conclusion drawn will be quite useful in helping to resolving the heat transfer and energy conversion problem during the miniaturization of integrated circuits and molecular electronics.