***Supplementary Material:***

**Investigation of Thermal Transport Properties in Pillared-Graphene Structure Using Non-Equilibrium Molecular Dynamics Simulations**

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**S1. Molecular Dynamics Simulations:**



Figure S1: The process of creating PGS and the graphene/CNT junction. (a) Graphene sheet is prepared by creating a hole that fits a (6,6) CNT. (b) (6,6) CNT is aligned with the hole in the graphene sheet in the manner shown. (c) the junction is created



Figure S2: (a) The hexagonal rings in the graphene/CNT junction and (b) the heptagonal ring in between the two hexagonal rings in the graphene/CNT junction

Table S1: System name, unit cell dimensions, volume, and number of carbon atoms per cell



Table S2: Simulation protocol for each of the simulated PGS systems



Table S3: Replication of simulated systems to get thermal conductivities along graphene and CNT

|  |  |  |
| --- | --- | --- |
| **System** | **Number of replications to get thermal conductivity along graphene (along x-axis)** | **Number of replications to get thermal conductivity along CNT (along z-axis)** |
| ALT\_IPD22.8830 | 6 | 6 |
| ZIG\_IPD29.8466 | 6 | 6 |
| ALT\_IPD30.3066 | 8 | 8 |
| ZIG\_IPD45.2925 | 8 | 8 |
| ALT\_IPD47.2896 | 10 | 10 |
| ZIG\_IPD68.0088 | 10 | 10 |

**S2. Results and Discussion:**



Figure S3: Cumulative heat flow in graphene and CNT in ALT\_IPD22.8830 system



Figure S4: Temperature profile of ALT\_IPD22.8830 PGS system. The temperature profile as shown is a function of structure length in Å (from heat source to heat sink). It can be observed that the steady state is reached in the unthermostated zones