

Abstract Submitted
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First-principles calculations of the phonon transport in carbon atomic chain systems based on atomistic Green's function formalism¹
HU SUNG KIM, YONG-HOON KIM, Graduate School of EEWS, Korea Advanced Institute for Science and Technology — We report on the phonon transport in carbon chain systems, and cumulene. We utilized first-principles calculation with localized atomic basis sets to calculate interatomic forces. Calculated phonon dispersion of polyynes and cumulene were well-matched with theoretical expectations. In addition, we considered the strain effect on the phonon properties of the carbon chain systems. The applied strain affected bond-length alternation (BLA) and force interaction range. Finally, even and odd carbon atomic chains bridging two zigzag graphene nanoribbons were investigated. Increase in the phonon contribution on thermal conductivity was found in case of even carbon chains with proper amount of strain.

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