

NT-P009

## First-principles Calculations of the Phonon Transport in Carbon Atomic Chains Based on Atomistic Green's Function Formalism

Hu Sung Kim<sup>1</sup>, Min Kyu Park<sup>2,3</sup>, Yong-Hoon Kim<sup>1</sup>

<sup>1</sup>Graduate School of EEWS, Korea Advanced Institute for Science and Technology, <sup>2</sup>Division of Industrial Metrology Korea Research Institute of Standard and Science, <sup>3</sup>University of Science and Technology

Thermal transport in nanomaterials is not only scientifically interesting but also technological important for various future electronic, bio, and energy device applications. Among the various computation approaches to investigate lattice thermal transport phenomena in nanoscale, the atomistic nonequilibrium Green's function approach based on first-principles density functional theory calculations appeared as a promising method given the continued miniaturization of devices and the difficulty of developing classical force constants for novel nanoscale interfaces. Among the nanomaterials, carbon atomic chains, namely the cumulene (all-double bonds,  $\cdots C = C = C = C \cdots$ ) and polyynes (alternation of single and triple bonds,  $\cdots C \equiv C - C \equiv C \cdots$ ) can be considered as the extreme cases of interconnection materials for nanodevices. After the discovery and realization of carbon atomic chains, their electronic transport properties have been widely studied. For the thermal transport properties, however, there have been few literatures for this simple linear chain system. In this work, we first report on the development of a non-equilibrium Green's function theory-based computational tool for atomistic thermal transport calculations of nanojunctions. Using the developed tool, we investigated phonon dispersion and transmission properties of polyethylene ( $\cdots CH_2 - CH_2 - CH_2 - CH_2 \cdots$ ) and polyene ( $\cdots CH = CH - CH = CH \cdots$ ) structures as well as the cumulene and polyynes. The resulting phonon dispersion from polyethylene and polyene showed agreement with previous results. Compared to the cumulene, the gap was found near the  $\Gamma$  point of the phonon dispersion of polyynes as the prediction of Peierls distortion, and this feature was reflected in the phonon transmission of polyynes. We also investigated the range of interatomic force interactions with increase in the size of the simulation system to check the convergence criteria. Compared to polyethylene and polyene, polyynes and cumulenes showed spatially long-ranged force interactions. This is reflected on the differences in phonon transport caused by the delicate differences in electronic structure.

**Keywords:** thermal transport, carbon chains, density functional theory, atomistic nonequilibrium Green's function

NT-P010

## Photodegradation of Volatile Organic Compound (VOC) Through Pure TiO<sub>2</sub> and V-Doped TiO<sub>2</sub> Coated Glasses

Jiyeon Moon, Seonmin Kim\*

Korea Electronics Technology Institute

TiO<sub>2</sub> possesses great photocatalytic properties but absorbs only UV light owing to high band gap energy ( $E_g = 3.2$  eV). By narrowing the band gap through doping a metal ion, the photocatalytic activity can be enhanced in condition of the light of a higher than 365 nm wavelength. Main purpose for this study is to evaluate the activities of metal doped TiO<sub>2</sub> for degrading the volatile organic compounds (VOCs); p-xylene is chosen in the VOC removal test. Vanadium is selected in this study because an ionic radius of vanadium is almost the same as titanium ion and vanadium can be easily doped into TiO<sub>2</sub>. V-doped TiO<sub>2</sub> was synthesized by sol-gel methods and compared with pure TiO<sub>2</sub>. Pure TiO<sub>2</sub> powder and V-doped TiO<sub>2</sub> powder were coated on glasses by spray coating method. UV-Visible spectrophotometer was used for the measurement of the band gap changes. VOC concentration degradation level was tested with using various UV light sources in an enclosed chamber. Catalytic activities of prepared samples were evaluated based on the experimental results and compared with coated pure TiO<sub>2</sub> sample.

**Keywords:** Titanium Dioxide, Volatile Organic Compound (VOC), Photocatalyst