

Abstract Submitted
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Computational Study of the Thermal and Electronic Transport Properties of Rigidly-Interconnected Carbon Nano Foam SORA PARK, YOUNG-KYUN KWON, Department of Physics and Research Institute for Basic Sciences, Kyung Hee University, DAVID TOMÁNEK, Physics and Astronomy Department, Michigan State University — We study the thermal and electronic transport properties of rigidly-interconnected structures having sp^2 carbon minimal surface called schwarzites. The system consists of core parts composed of schwarzite and interconnection parts with (4,4) carbon nanotube segments [1]. Using direct molecular dynamics simulations with the Tersoff potential, we compute the thermal conductivity of various configurations to explore the dependence on the number of core parts and on the length of interconnection parts. Our calculations show that each core part plays as a scattering center, which reduces the phonon mean free path and thus the thermal conductivity. We also investigate the electronic transport properties of the system by applying the non-equilibrium Green function approach in combination with density functional theory. We explore the effects of different core connectivity and structural defects introduced near the core parts on the electrical conductance. These thermal and electronic properties may be connected to the thermoelectric properties of the schwarzite system.[1] S. Park, K. Kittimanapun, J. S. Ahn, Y.-K. Kwon and D. Tománek, J. Phys.: Condens. Matter **22**, 334220 (2010).

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