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Study of percolation behavior depending on molecular structure design JI WOONG YU, WON BO LEE, School of Chemical and Biological Engineering, Seoul National University, Seoul 08826, Republic of Korea — Each differently designed anisotropic nano-crystals(ANCs) are studied using Langevin dynamic simulation and their percolation behaviors are presented. Popular molecular dynamics software LAMMPS was used to design the system and perform the simulation. We calculated the minimum number density at which percolation occurs(i.e. percolation threshold), radial distribution function, and the average number of ANCs for a cluster. Electrical conductivity is improved when the number of transfers of electrons between ANCs, so called "inter-hopping process", which has the considerable contribution to resistance decreases and the number of inter-hopping process is directly related with the concentration of ANCs. Therefore, with the investigation of relationship between molecular architecture and percolation behavior, optimal design of ANC can be achieved.

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