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Electron Trapping and Transport in Poly(tetraphenyl)silole Siloxane of Quantum Well Structure

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A new kind of organic-inorganic hybrid polymer, poly(tetraphenyl)silole siloxane (PSS), was invented and synthesized for realization of its unique charge trap properties.[1] The organic portions consisting of (tetraphenyl)silole rings are responsible for electron trapping owing to their low-lying LUMO, while the Si-O-Si inorganic linkages of high HOMO-LUMO gap provide the intrachain energy barrier for controlling electron transport. Such an alternation of the organic and inorganic moieties in a polymer may give an interesting quantum well electronic structure in a molecule. The PSS thin film was fabricated by spin-coating of the PSS solution in THF organic solvent onto Si-wafer substrates and curing. The electron trapping of the PSS thin films was confirmed by the capacitance-voltage (C-V) measurements performed within the metal-insulator-semiconductor (MIS) device structure. And the quantum well electronic structure of the PSS thin film, which was thought to be the origin of the electron trapping, was investigated by a combination of theoretical and experimental methods: density functional theory (DFT) calculations in Gaussian03 package and spectroscopic techniques such as near edge X-ray absorption fine structure spectroscopy (NEXAFS) and photoemission spectroscopy (PES). The electron trapping properties of the PSS thin film of quantum well structure are closely related to intra- and inter-polymer chain electron transports. Among them, the intra-chain electron transport was theoretically studied using the Atomistix Toolkit (ATK) software based on the non-equilibrium Green's function (NEGF) method in conjunction with the DFT.

1. Jin-Kyu Choi, Seunghyun Jang, Ki-Jeong Kim, Honglae Sohn, and Hyun-Dam Jeong J. Am. Chem. Soc. 2011, 133, 7764.

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