ナノ空間を主導パラメータとする量子ドット結晶の計算科学的デザイン

Computational Designs of Quantum Dot Superlattice Characterized by Hyper-Nano Space

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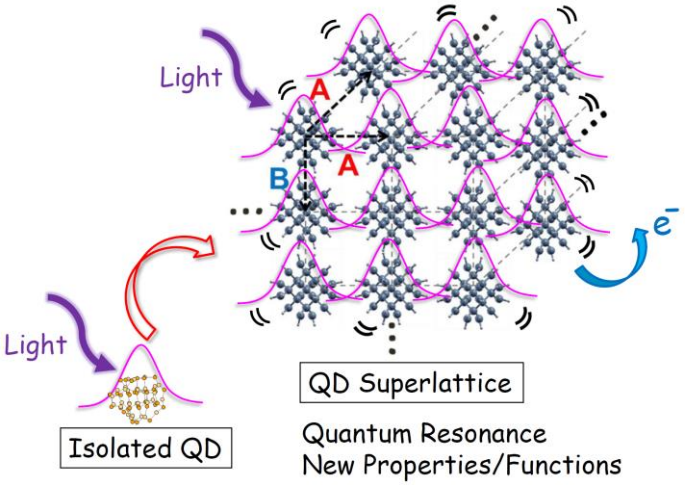

Quantum dot (QD) superlattice, a periodically ordered array structure of QDs, is expected to provide novel photo-optical functions owing to resonant couplings between adjacent QDs. [1] We computationally demonstrated that electronic structures and phonon dynamics of QD superlattice can be effectively and selectively controlled by manipulating its interior nano space where quantum resonance between neighboring QDs appears rather than by changing component QD size, shape, compositions, etc. [2] A simple H-passivated Si QD was examined to constitute one-, two- and three-dimensional QD superlattice, and thermally fluctuating band energies and phonon modes were simulated by finite-temperature ab initio molecular dynamics (MD) simulations. The QD superlattice exhibited decrease of the band-gap energy enhanced by thermal modulations and also selective extraction of charge carriers out of the component QD, indicating its advantage as a promising platform to be implemented in solar cells. Our dynamical phonon analyses based on the ab initio MD simulations revealed that THz-frequency phonon modes were created by inter-QD crystalline lattice formed in the QD superlattice, which can contribute to thermoelectric conversion of low energy and will be useful for direct observation of the dimension-dependent superlattice. Further, we found that crystalline and ligand-originated phonon modes inside each component QD can be independently controlled by asymmetry of the superlattice and by restriction of the interior nano space, respectively. Taking into account the thermal effects at the finite temperature, we will propose guiding principles for designing efficient and space-saving QD superlattice to develop functional photovoltaic and thermoelectric devices. We will also briefly report photoexcited dynamics taking place in QD superlattice and discuss its difference from the isolated QD case. [3]

[1] D. Kim, S. Tomita, K. Ohshiro, T. Watanabe, T. Sakai, I.-Y. Chang and K. Hyeon-Deuk, *Nano Letters* **15** (2015) 4343.
[2] I.-Y. Chang, D. Kim and K. Hyeon-Deuk, *ACS Applied Materials & Interfaces* (2016) in press.
[3] submitted.

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