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Manipulation of Energy Gap of Thallium Quantum Dots

CHOONGYU HWANG, NAMDONG KIM, GEUNSIK LEE, SUNYOUNG SHIN, SANGHUN UHM, HYOSANG KIM, JAESAM KIM, JINWOOK CHUNG, Physics, POSTECH — We have characterized the electronic properties of thallium (Tl) quantum dot (QD) array using high-resolution electron-energy-loss spectroscopy, photoemission spectroscopy, and first-principle calculations. The surface with the QD's exhibits a weakly semiconducting character with a band gap less than 0.23 eV in sharp contrast with previous scanning-tunneling spectroscopy observation [1]. We have observed the non-varying excitation energy of an interband transition in conflict with two kinds of binding energy shift with the variation of effective separation between the QD's. We analyze the experimental findings through first-principle calculations based on the density functional theory using ab initio plane wave pseudo-potential method within generalized-gradient approximations. Nine Tl atoms are found to form a QD occupying the attractive basin around the Si restatoms in the faulted half unit cell and the surface is semiconductor with an energy gap of 0.11 eV. The calculated band structure of Tl QD's shows the bonding origin of surface states, confirming our experimental results. The origin of the difference in binding energy shift of each electron state is the interaction between electrons only in QD's, leaving the electron states irrelative to QD's unshifted. [1] L. Vitali, M. G. Ramsey, and F. P. Netzer, Phys. Rev. Lett. 83, 316 (1999).

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