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Phonon-induced superlattice structures in titanium-oxypnictides superconductors KENTA HONGO, KOUSUKE NAKANO, RYO MAEZONO, Japan Adv Inst of Sci and Tech — First-principles electronic and phonon simulations have been carried out within density functional theory (DFT) for layered titanium-oxypnictides, $BaTi_2Pn_2O$ (Pn = As, Sb, Bi). We have found a new possibility of orthorhombic $2 \times 2 \times 1$ superlattice structure for $BaTi_2As_2O$, while that of tetragonal $\sqrt{2} \times \sqrt{2} \times 1$ for $BaTi_2Sb_2O$ and $BaTi_2Bi_2O$ [1]. It was found that their phonon dispersons and changes of nesting vectors in Fermi surfaces can account for such varieties of superlattice structures even starting with the common undistorted structure when without the charge ordering. This new finding can naturally resolve a discrepancy between experiments and theoretical predictions on the charge ordering of the compounds without any relying on complicated unconventional mechanism proposed recently, which could also affect the understanding of superconductivity on the compounds. [1] K. Nakano, K. Hongo, and R. Maezono, Sci. Rep. 6, 29661 (2016).

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