**New One-Dimensional Material Nb2Se9: Theoretical Prediction of Indirect to Direct Band Gap Transition Due to Dimensional Reduction**

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Dimensionality reduction of some two-dimensional transition metal chalcogenides can produce direct band gap where three-dimensional structure shows indirect band gap. Recently, Nb2Se9 is made as 1-dimensional structure by solid state reaction. This is composed of periodically stacked single-chain atomic crystals (SCAC) where the SCACs form inorganic bulk crystals due to strong bonds within the chain but weak inter-chain interactions. To find whether the band gap transition is occurred in this SCAC materials, the band structures of Nb2Se9 SCACs composed of 1-7 single chains is calculated using density functional theory. Unlike the bulk structure of Nb2Se9, that chain bundles composed of up to 21 single SCACs would have a direct band gap. Band gap increase as the number of chains in the bundle decreased. Accordingly, Nb2Se9 bundle SCAC with a diameter of 3.6 nm is expected that it can cause the electronic transition without being disturbed by the phononic environment due to the direct band gap, and can be used in photoluminescence applications.