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Intrinsic charge transport in stanene: Role of buckling and electron-phonon coupling

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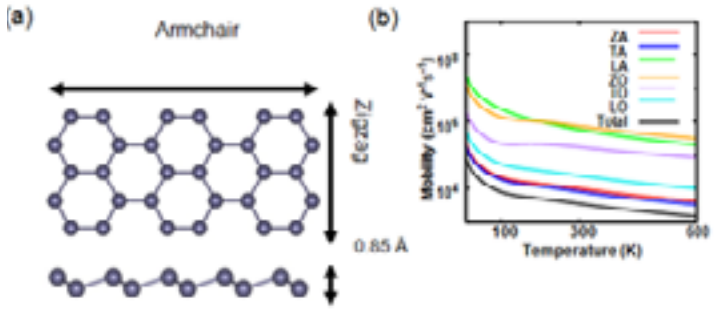
Among two-dimensional materials, group IV elemental sheets such as graphene, silicene, germanene and stanene have been intensively investigated using first principles calculation. We look at the intrinsic carrier mobility for stanene, or the tin-monolayer, using Boltzmann transport equation coupled with density functional perturbation theory plus Wannier interpolation approximation to consider electron scattering with all the phonon branches with dispersion contribution. It is found that the conventional deformation potential (DP) approach which worked well for many layered materials, can well overestimate the carrier mobility in stanene because the buckled structure allows more types of electron-phonon scattering, such as acoustic flexural mode. DP theory assumed that only longitudinal acoustic phonon in long wavelength limit ($|q|<0$) contributes to the charge relaxation process. In this work, we calculate all phonon modes, such as out-of-plane acoustic mode, transverse acoustic mode, and optical counterparts, in addition to longitudinal acoustic mode, plus dispersion effects and we investigate the intrinsic carrier mobility, in comparison with the DP theory. We find that the intrinsic carrier mobility could be as high as $2\sim3\times10^6$ cm^2 V^{-1} s^{-1} by DP theory but becomes only $2\sim3\times10^3$ cm^2 V^{-1} s^{-1} by the full evaluation of electron-phonon coupling. It is found that the intervalley scattering process in acoustic out-of-plane and transverse mode, which DP ignored dominate the carrier relaxation.



Biography

Yuma Nakamura is now pursuing two Master degrees in the Department of Chemistry, Tsinghua University, China and Department of Physics, Tohoku University, Japan in double degree program. He received his BSc (2015) in the Department of Physics, Tohoku University. He has worked as a Reviewer of peer reviewed *Journal of Material Research*. His research interest covers computational chemistry, two-dimensional materials, and charge and spin transport phenomena. He has his expertise in density functional theory (DFT) and density functional theory (DFPT) for simulating material property.

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