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First-principles calculation of the heat transport properties of strained graphene nanoribbons CHEE KWAN GAN, Institute of High Performance Computing, Singapore, PEI SHAN EMMELINE YEO, National University of Singapore — We use density-functional theory coupled with a nonequilibrium Green function's method to calculate the characteristics of ballistic thermal transport (P.S.E. Yeo, K.P. Loh, and C.K.Gan, Nanotechnology, 2012, accepted and to appear) of tensile-strained armchair (AGNR) and zigzag (ZGNR) edge graphene nanoribbons, with widths between 3 and 50 Å. The optimized lateral lattice constants for AGNRs of different widths display a three-family behavior when the ribbons are arranged according to N modulo 3, where N represents the number of carbon atoms across the width of the ribbon. Two lowest-frequency out-of-plane acoustic modes play an important role in increasing the thermal conductance of AGNR-N at low temperatures. At high temperatures the effect of tensile strain is to reduce the thermal conductance of AGNR-N and ZGNR-N. These results could be explained by the changes in force constants in the in-plane and out-of-plane directions when strain is applied. This fundamental atomistic understanding of the heat transport in graphene nanoribbons suggests a route to controlling heat transport properties via strain at various temperatures.

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