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Tunable thermal transport and negative differential thermal conductance in graphene nanoribbons JIUNING HU, YAN WANG, AJIT VALLABHANENI, XIULIN RUAN, YONG CHEN, Purdue University — We have studied thermal transport in graphene nanoribbons (GNRs) using classical nonequilibrium molecular dynamics simulations. We show that the calculated thermal conductivity of GNRs can be dramatically tuned by the shape, isotope composition, defects, and chirality and hydrogen passivation of the edges [1-2]. For GNRs under large temperature bias beyond the linear response, we have studied negative differential thermal conductance (NDTC) [3]. The NDTC is found to vanish for a sufficiently long GNR whose temperature is fixed at one end. Furthermore, for diffusive thermal transport obeying differential Fourier's law in a generic one-dimensional system, we analytically show that NDTC requires temperature dependent thermal conductivity and simultaneously varying temperatures at both ends. We have also studied asymmetrical GNRs and observed thermal rectification [1] and direction dependent NDTC [3]. Our studies may be useful for nanoscale thermal managements and thermal signal processing using GNRs and understanding low dimensional thermal transport in general.

[1] J. Hu et. al., Nano Letters 9, 2730 (2009)

[2] J. Hu et. al., Applied Physics Letters 97, 133107 (2010)

[3] J. Hu et. al., Applied Physics Letters 99, 113101 (2011)

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