Phonon thermal transport in 2H, 4H and 6H silicon carbide from first principles NAKIB PROTIK, Boston College, ANKITA KATRE, CEA-Grenoble, LUCAS LINDSAY, Oak Ridge National Laboratory, JESUS CARRETE, CEA-Grenoble, B. DONGRE, G.K.H. MADSEN, Technical University of Vienna, NATALIO MINGO, CEA-Grenoble, DAVID BROIDO, Boston College — Silicon carbide (SiC) is widely used in electronic devices, in part because its high thermal conductivity helps prevent ‘hot spots’ to maintain uniform device operating temperatures. Here we present ab initio calculations of the in-plane and cross-plane thermal conductivities, \( k_{\text{in}} \) and \( k_{\text{out}} \), of the hexagonal SiC polytypes, 2H, 4H and 6H. These calculations combine a full solution of the phonon Boltzmann equation with accurate determination of interatomic force constants from density functional theory. Generally, \( k_{\text{out}} \) values are found to be smaller than \( k_{\text{in}} \) values for a given polytype. Both \( k_{\text{in}} \) and \( k_{\text{out}} \) decrease with increasing \( n \) in \( n \)-H SiC. This finding is contrary to previous measurements, which showed 4H SiC having lower \( k \) than 6H SiC [1]. Specific comparisons will be made to existing measured and calculated results. We will also discuss the formation of defects, and their effect on thermal conductivity. [1] D. T. Morelli, J. P. Heremans, C. P. Beetz, W. S. Yoo, and H. Matsunami, Appl. Phys. Lett. 63, 3143 (1993); Rusheng Wei, et al., J. Appl. Phys. 113, 053503 (2013).