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Thermal conductivity of one-, two- and three-dimensional sp2 carbon LUIZ FELIPE PEREIRA, Max Planck Institute for Polymer Research, Mainz, Germany, IVANA SAVIC, Tyndall National Institute, Cork, Ireland, DAVIDE DONADIO, Max Planck Institute for Polymer Research, Mainz, Germany — Carbon atoms can form structures in one, two and three dimensions due to their unique chemical versatility. In terms of thermal conductivity, carbon polymorphs cover a wide range from very low values with amorphous carbon to very high values with diamond, carbon nanotubes and graphene. Schwarzites are a class of three-dimensional fully covalent sp2-bonded carbon polymorphs, with the same local chemical environment as graphene and carbon nanotubes, but negative Gaussian curvature. We calculate the thermal conductivity of a (10,0) carbon nanotube, graphene and two schwarzites with different curvature, by molecular dynamics simulations based on the Tersoff empirical potential. We find that schwarzites present a thermal conductivity two orders of magnitude smaller than nanotubes and graphene. The reason for such large difference is explained by anharmonic lattice dynamics calculations, which show that phonon group velocities and mean free paths are much smaller in schwarzites than in nanotubes and graphene. Their reduced thermal conductivity, in addition to tunable electronic properties, indicate that schwarzites could pave the way towards all-carbon thermoelectric technology with high conversion efficiency.

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