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Largely tunable anisotropic thermal conductivity of pristine and lithiated MoS2 SHUNDA CHEN, Univ of California - Davis, ADITYA SOOD, ERIC POP, KENNETH GOODSON, Stanford University, DAVIDE DONADIO, Univ of California - Davis — Understanding heat transport in two-dimensional (2D) layered materials is of importance for potential applications in energy storage, nanoelectronics and optoelectronics. The vibrational properties of 2D layered materials could be tailored in several different ways either by chemical modifications or mechanically. Here we investigate heat transport in MoS2, upon lithium intercalation and cross-plane strain, by first principles calculations. We find that both the in-plane and cross-plane components of the thermal conductivity of MoS2 are extremely sensitive to both strain and electrochemical intercalation. Furthermore, since in-plane thermal conductivity and cross-plane thermal conductivity respond in different ways to intercalation and strain, the thermal conductivity anisotropy can be modulated over two orders of magnitude. The underlying mechanisms for such large tunability of the anisotropic thermal conductivity of MoS2 are explored by computing phonon dispersion relations, relaxation time and mean free paths. Since both intercalation and strain can be applied reversibly their stark effect on the thermal conductivity can be exploited to design novel phononic devices, as well as for thermal management in MoS2-based electronics and optoelectronic systems.

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