MELoDICA: Disclosing the potential of transition metal dichalcogenides for thermoelectric applications through nanostructuring and confinement

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Abstract

Transition metal dichalcogenides (TMDs) offer a huge flexibility in tuning electronic properties, indeed, their electronic structure is found to change dramatically from bulk to few monolayers samples. Moreover, some TMDs exhibit potentially remarkable bulk thermoelectric (TE) behavior, which may be further improved in few monolayers thick nanostructures, according to theoretical predictions. On the other hand, TMD flakes can be produced by liquid phase exfoliation of their bulk counterpart by using scalable and cheap methods and restacked nano-flake assemblies may offer ideal nanostructured morphology that effectively scatters phonon of different wavelengths, thus suppressing lattice thermal conductivity, typically in the range of tens Wm-1K-1 at room temperature in single flakes, and improving TE performances. The aim of our proposal is to explore the potential of these features – i.e. electronic confinement and nanostructured morphology - in view of enhanced TE performance of these systems for applications in energy conversion. We will prepare TMDs (e.g. MoTe2, ZrSe2, MoS2, MoSe2, WSe2, WTe2, HfSe2, SnSe2, HfTe2 …) in different forms, namely bulk single crystals, epitaxial ultrathin films and heterostructures (grown by molecular beam epitaxy), nanoflakes (obtained by liquid phase exfoliation and subsequent ink-jet printing and drop-casting). In these samples, we will measure electric, thermoelectric and thermal transport properties. In TMD ultrathin films and heterostructures, we will focus on the possibility of tuning TE properties via thickness. In assembled flake patterns, we will further explore the effect of confinement, but also address phonon engineering by nanostructural configurations, in terms of suitable distribution of thickness and size, as well as proper inter-flake connectivity. In parallel, deeper insight will be gained by carrying out theoretical calculations of electric, thermoelectric and thermal transport properties, focusing on the effects of confinement and presence of interface thermal resistances.Our investigation starts from the optimization of the sample preparation processes and it proceeds by combining experimental measurements and theoretical calculations, eventually aiming to obtain a comprehensive understanding of the physical mechanisms into play and a realistic assessment of TMDs as TE materials for device applications such as TE micro-coolers, on the basis of our own experimental results, as well as of the estimated edge of improvement possibly yet achievable.

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