NANOTECHNOLOGIES

UTAustin Portugal

Non-equilibrium heat and charge transport in nanocrystal superlattices: *in silico* study

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Background

This work is a part of ongoing UT Austin-Portugal project "UT-BORN-PT: Unconventional Thermoelectrics Based on Self-Organized Binary Nanocrystal Superlattices". It aims to increase thermopower *S* due to band engineering, along with decreasing thermal conductivity via phonon scattering, improving thermoelectric efficiency η.

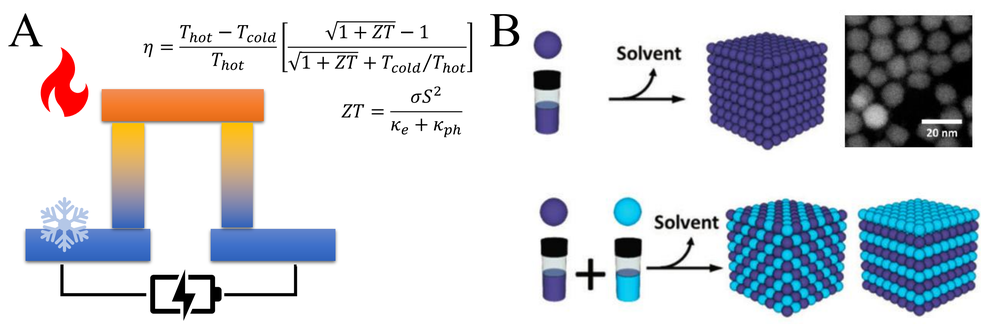
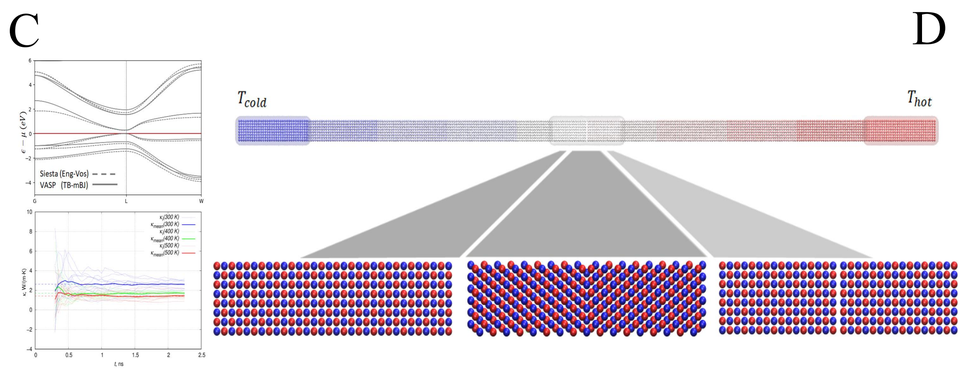


Figure B: Superlattice self-assembly from Ortega S, et al. Chem Soc Rev. 2017;46(12):3510–28; Inset from Piotrowski M, et al. J Phys Chem C 2018;122(48):27127–34

Methodology

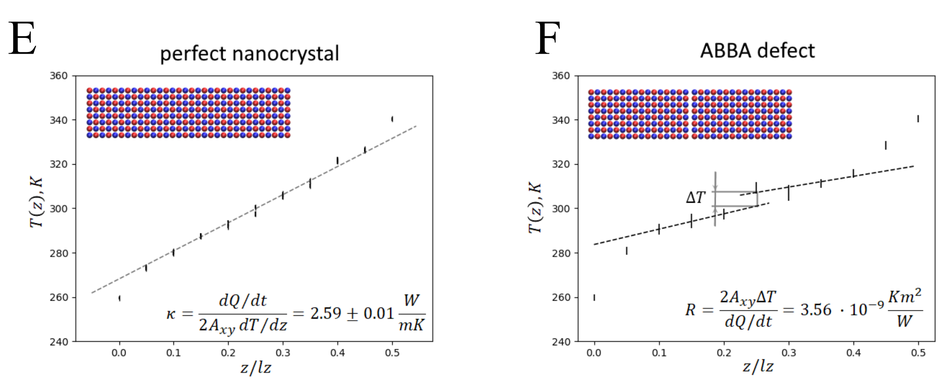
We use non-equilibrium molecular dynamics and density functional theory calculations to study scattering of phonons and electrons by various interfaces. To model PbTe on a large scale we use Buckingham pair-potentials[1] and Engel-Vosko XC functional[2], proven to give good agreement with more precise methods within the ϵ and *T* range of interest.



1. Qiu B, Bao H, Zhang G, Wu Y, Ruan X. Comput Mater Sci. 2012;53:278–85.
2. Kim H, Kaviany M. Phys Rev B. 2012;86:45213.

Preliminary results

Figures E and F shows profiles of temperature variations for chunks of 2048 atoms along thermal transport directions. Linear fit for perfect PbTe crystal (fig. E) gives acceptable agreement with known experimental value of $\kappa \sim 2.8 \frac{W}{m \cdot K}$. Fig. F shows a temperature drop resulting plane defect, imitating one of possible interface conditions.



Impact/Conclusions

Currently available methods allow us to extract bulk and interface thermal and electric conductivities on a scale comparable with size of nanoparticles used in experiments without sacrificing atomic scale details, such as interface structure.

This project is still the work in progress. The approach is now generalized for heterogeneous interfaces, including different types of surface passivation. The estimated interface thermal and electric resistances will be later integrated into a mesoscale model to study the effect of superlattice packing.

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