Thermal and Thermoelectric Transport in Polymers

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Thermal transport in polymers is a fascinating area of research as experimental observations are not well described by existing transport models. For example, the thermal conductivity of polymers at low temperatures (~1-200 K) exhibit characteristics of propagons and diffusons as qualitatively described by Allen and Feldman,[1] and are not well described by the k-min or the Einstein models.[2] To better understand thermal conductivity in polymers, an empirical model was developed based on the concept of propagons and diffusons, which can be surprisingly predictive using the correlations to other material properties (monomer molecular weight, density, and speed of sound).[3] This model can also parse the contributions from both extended vibrational modes and diffusive like modes, which could influence the electronic and thermoelectric transport in polymers at different length scales. Also, this empirical model predicts an upper limit on the amorphous thermal conductivity from propagon and diffuson contributions, suggesting that locon contributions and/or crystallinity are necessary to exceed this limit in route to thermally conducting polymers.

The thermoelectric transport in polymers is also a fascinating area of research as electronic and thermoelectric transport models that better describe the experimental observations are currently ongoing. It is only recently that thermoelectric properties of these materials have been measured. Currently there are only a couple models emerging to describe the experimental observations between electrical conductivity and thermopower.[4] Moreover, while a great deal of research has already been undertaken on p-type polymers, little research into n-type thermoelectric polymers has taken place. This is primarily because many of the existing n-type polymers are not air stable. For this reason, we have been exploring organometallic polymers (*i.e.*, metal-coordinated polymers), which are air stable.[5] While we currently do not have an explanation, we observe a correlation between the sign the of the Seebeck coefficient of the bulk metal and the metal center in the polymer; for example, Ni containing polymers have negative Seebeck coefficients where Pt containing polymers have positive Seebeck coefficients.

This presentation will touch on both thermal transport in polymers and thermoelectric transport in n-type organometallic polymers. This talk will serve as an introduction into these two areas identifying interesting experimental observation and our attempts to understand transport in these systems so we can make predictions that may influence future research directions.

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