

To investigate potential implementation in thermal energy storage and harvesting applications, we show that the Al JDTD enables a half-wave thermal rectifier circuit that rectifies time-periodic temperature profiles, achieving thermal circuit effectiveness values up to 30 % of the ideal-diode limit at rectification ratios near 5. When coupled with thermal capacitances, such time-periodic thermal rectification could aid cold energy storage for passive cooling of components subjected to time-periodic thermal boundary conditions. Thus, our findings showcase the functionality of Al-based surfaces for thermal rectification and could guide future work aiming to apply Al JDTDs for improved thermal management.

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5:00 PM EN07.05.12

Effect of Fluorination on The Thermal Conductivity of Graphite Fluoride (CF) Wonsik Lee, Seungbin Han and Hyejin Jang; Seoul National University, Korea (the Republic of)

For thermal management applications, there are surging demands for materials with high thermal conductivity and electrically insulating properties. Graphite fluoride (CF), one of the novel graphene-based layered materials, has emerged as a promising thermal management material owing to its similar crystal structure to that of graphite yet electrically insulating properties, i.e., electronic band gap of over 3 eV. CF is expected to show high thermal conductivity due to its structural similarity to graphite. However, the degree of which fluorination alters the thermal conductivity is largely unexplored, and even the thermal conductivity is not experimentally established. Here, we report the through- and in-plane thermal conductivity of mechanically exfoliated CF flakes for the first time by using time-domain thermoreflectance (TDTR). At room temperature, a 70-nm-thick CF flake shows $(1700 \pm 300) \text{ W m}^{-1} \text{ K}^{-1}$ for in-plane direction, which is about 90 % of that of graphite, and $(4.0 \pm 0.8) \text{ W m}^{-1} \text{ K}^{-1}$ for through-plane direction. The through-plane thermal conductivity of CF flakes shows quasi-ballistic behavior for thicknesses $< 200 \text{ nm}$, which is similarly observed in graphite but shows two times higher through-plane thermal conductivity than that of graphite. We calculate the phonon properties of monolayer graphene and graphene fluoride to reveal the intrinsic phonon transport mechanisms by solving the phonon Boltzmann transport equation (BTE). BTE estimates the thermal conductivity of graphene and graphene fluoride as $3000 \text{ W m}^{-1} \text{ K}^{-1}$ and $270 \text{ W m}^{-1} \text{ K}^{-1}$, respectively. Phonon mode thermal conductivity indicates that the fluorination opens an out-of-plane acoustic (ZA) phonon scattering channel and the ZA phonon contribution to the thermal conductivity of CF is greatly suppressed, compared to the case of graphene. To understand the discrepancy in thermal conductivity between the experimental and theoretical results, we characterize the chemical and optical properties of exfoliated CF flakes to correlate those properties with thermal conductivity results. We believe this work reveals the role of functional groups on thermal conductivity in graphene/graphite-derivative materials.

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Impact of Cooling Rate and Thermal Mass on Supercooling in a Salt-Hydrogel Complex for Thermal Energy Storage Youngmun Lee, Daniel Hsieh, Sung Bum Kang, Paul V. Braun and Sanjiv Sinha; University of Illinois at Urbana Champaign, United States

Glauber's salt is a promising phase change material for building thermal management because of its high latent heat, acceptable melting temperature of 32.3°C for indoor air^{1,2}. Despite these advantages, the practical application of Glauber's salt in thermal energy storage systems is still challenging due to supercooling and phase segregation¹⁻³. Here, we report the impact of temperature ramp rate and thermal mass on the supercooling of Glauber's salt through the DSC and T-history experiment. The ramp rate effect was studied with a wide range of ramp rates in 1 to 10°C/min in DSC and 1 to 4°C/min in the T-history experiment. The thermal mass effect was investigated by comparing DSC and T-history experiment. The latent heat was also analyzed for different ramp rates and thermal mass conditions. The melting temperatures of Glauber's salt from the two techniques were identical while freezing temperatures were different because of the thermal mass effect. During freezing in the T-history experiment, the latent heat was reduced by around 75% to the latent heat in melting due to supercooling and phase segregation. To overcome this bottleneck, we developed a novel hydrogel complex that reduces the supercooling and prevents phase segregation to maintain volumetric energy density for 100 cycles. Thermodynamic analysis accounting for composition shows that a higher salt composition can further enhance the volumetric energy storage density. For example, a 10% increase in the weight percentage of salt leads to about 50% enhancement in volumetric energy storage density.

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5:00 PM EN07.05.16

Supramolecular Interactions lead to Remarkably High Thermal Conductivities in Interpenetrated Two Dimensional Porous Crystals Jaymes Dionne¹, Ashutosh Giri¹ and Patrick E. Hopkins^{2,2,2}; ¹University of Rhode Island, United States; ²University of Virginia, United States

The design of innovative porous crystals with high porosities and large surface areas has garnered a great deal of attention over the past few decades due to their potential for a variety of applications, including flexible electronics, gas storage, and catalysts, among others. However, heat dissipation poses a major challenge in porous crystals and enhancing heat dissipation is key to realizing their potential. In this work, we use systematic atomistic simulations to show that the interpenetration of two, two-dimensional frameworks possess remarkable thermal conductivities at high porosities compared with their single three-dimensional framework and interpenetrated three-dimensional framework counterparts. Typically, high thermal conductivities are associated with low porosities; however, this work provides an alternative method to retain high porosities while drastically enhancing the thermal conductivity of the porous crystal. We attribute this to lower phonon-phonon scattering and vibrational hardening from supramolecular interactions that restrict atomic vibrational amplitudes, enhancing heat conduction. We also show this for realistic systems, with a two-dimensional interpenetrated framework of COF-1 achieving an order of magnitude increase in thermal conductivity when compared to its three-dimensional counterpart, COF-300. This introduces a new