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Interfacial Thermal Transport in Energy and Environmental Applications

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Interfacial thermal transport at the nanoscale is critical in a wide variety of applications such as electric device,[1] energy storage,[2] biomedical devices,[3] optoelectronics,[4] etc. Despite the thermal transport across the interface is becoming more critical when the characteristic dimensions of the system reach the nanometer scale,[5] the current fundamental understanding of the interfacial thermal transport is still far from complete. Different types of interface thermal transport exist in various applications, there is mainly solid-solid and solid-liquid interfacial thermal transport (see in Figs. 1a~b). Phonon vibrational mismatch or surface roughness can partially explain the nanoscale solid-solid interface thermal transport,[6] however, for solid-liquid or solid-gas interface thermal transport, the definition of phonons for liquids remains questionable due to the lack of periodicity. In this short editorial, we review the current state of the field of interfacial thermal transport in energy and the environmental applications which involved interfacial thermal transport and provide our perspectives on the challenges and the remained questions.

Experimental studies of interfacial thermal transport are methodologically limited at the nanoscale. Optothermal method based on the Raman spectroscopy[7,8] is widely used but the calibration of temperature/power is time-consuming and the laser absorption can be difficult to decide which can further lead to more uncertainties.[9] Computational methods, on the other hand, such as molecular dynamics,[10] lattice dynamics[11] can provide more physical insight and vivid microscopic images which is helpful to investigate the mechanism of interfacial thermal transport but the force field needs to be chosen carefully for specific molecular systems. Moreover, relevant physical models and theories are employed to calculate the thermal properties and reveal the transportation mechanism. However, a gap between the simulation and experiment results always exits and more novel experimental methods and the large-scale simulations are the next steps to reduce these gaps.

In the energy storage field, solid-state lithium-ion batteries (SLIBs) are the desired applications to meet the increasing energy and power demand due to their higher energy and power density.[12] However, with such high energy density, SLIBs face the critical problem of heat dissipation. The studies of interfacial thermal transport at the interface of electrodes materials and between electrode material and electrolyte are vital to the thermal management of SLIBs. Heterostructures are one of the most promising electrode material.[13] The addition of heterostructure (graphene, boron nitride, nitrogen-doped graphene) not only increases the cycle life of the battery but also improves heat dissipation.[14](Fig. 2). Many factors affect the interfacial thermal transport of heterostructures, including interlayer distance, coupling factor, temperature, size, strain, *etc*. The fascinating point about heterostructures is that the thermal properties of the material can be tuned by nanoengineering. For example, the interlayer distance can be altered by doping and surface chemical modifications, leading to changes in the thermal properties of the interface.[15] New ideas are constantly proposed, such as interference methods based on the wave nature of phonons, which contribute to the deep regulation of the thermal properties of materials. The interfacial thermal transport between electrodes and electrolytes of more different materials needs to be studied since each interface is unique and different heat energy carriers might exist due to such complex interfacial interplay.

Solar energy is the regenerated, green, abundant, and most accessible source of energy to combat pressing global warming and environmental issues. Sunlight can be absorbed directly by working fluids called nanofluids through photothermal interaction that has gained tremendous growth and widespread interest.[16] The interfacial thermal properties of nanoparticle and based fluids play a significant role in the overall thermal properties of the nanofluids. Common

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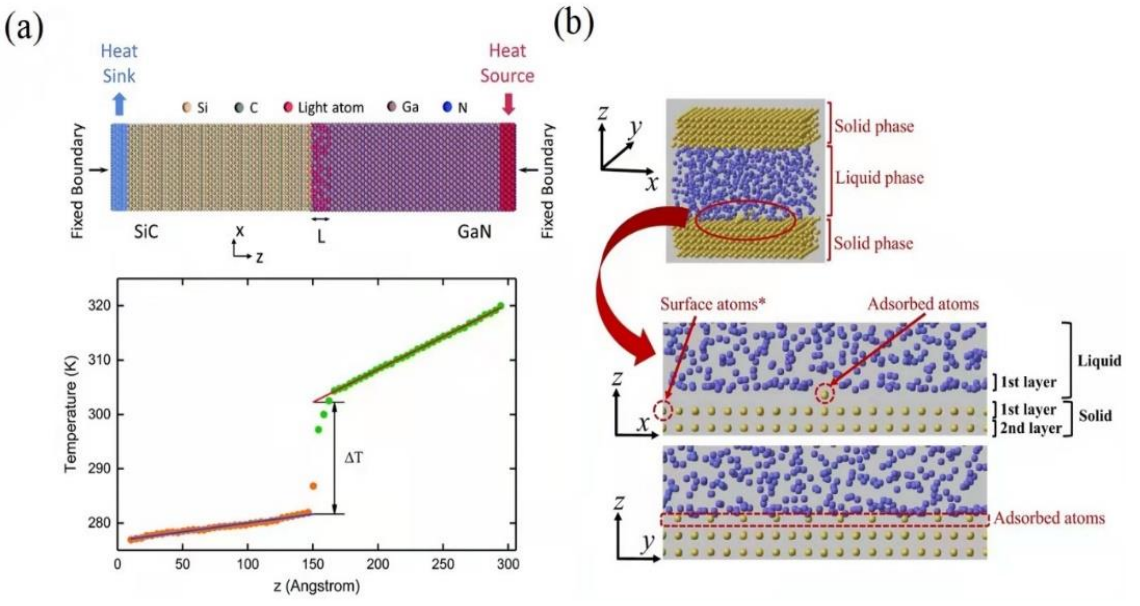

Fig. 1 Schematic diagram of a. solid-solid interface. Reproduced with the permission from [23], Copyright Royal Society of Chemistry (Physical Chemistry Chemical Physics). b) solid-liquid interface. Reproduced with the permission from [24], Copyright Springer Nature Scientific Report.

nanofluids include water-nanotube nanofluid,[17] oil-Cu nanofluid,[18] ethylene glycol-graphene nanofluid,[19] *etc*. Thermal transport across the solid-liquid interface strongly depends on the interfacial layer which is an ordered liquid layer cover on the solid surface. Numerous models and methods, such as the acoustic mismatch model (AMM) and molecular dynamics have been used to investigate the interfacial layer. However, these analyses can only be performed for specific systems. An analytical model which can be widely applied to various nanofluid interfacial layers is still needed.

For environmental applications, solar-driven water evaporation is a sustainable and green method to satisfy the demand of scarcity of water resources and environmental

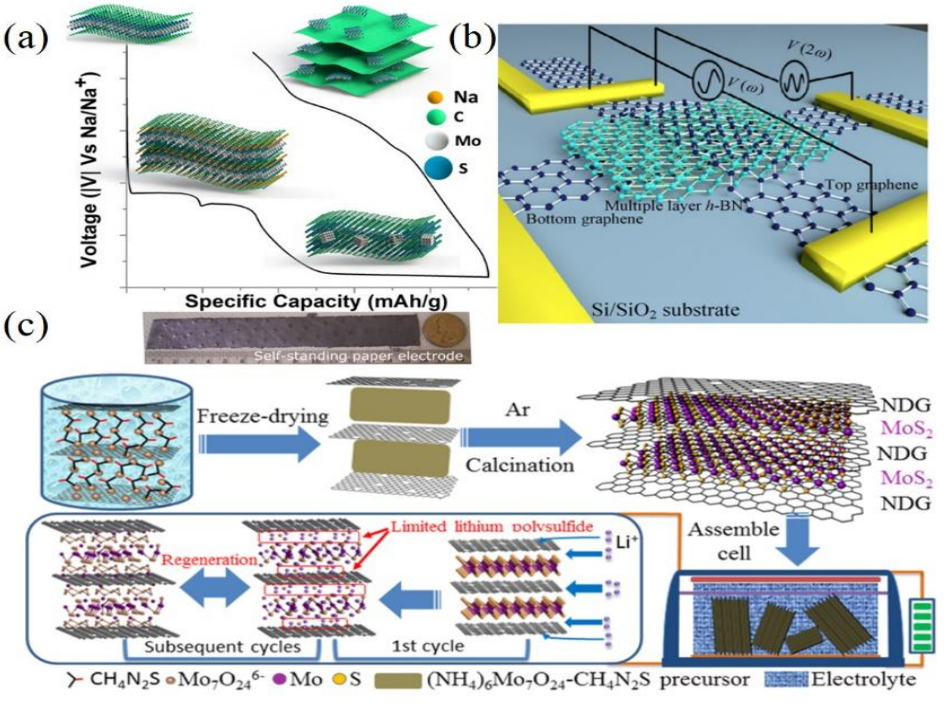

Fig. 2 a) Graphene oxide/MoS_2 flakes for sodium-ion batteries. Reproduced with the permission from [25], Copyright American Chemical Society ACS Nano, **b)** Schematic diagram of graphene/h-BN/graphene/Al_2O_3 heterostructure. Reproduced with the permission from [26], Copyright Springer Nature Nano Research, c) Preparation of nitrogen-doping graphene/MoS_2/ nitrogen-doping graphene heterostructure. Reproduced with the permission from [27], Copyright Elsevier Nano Energy.

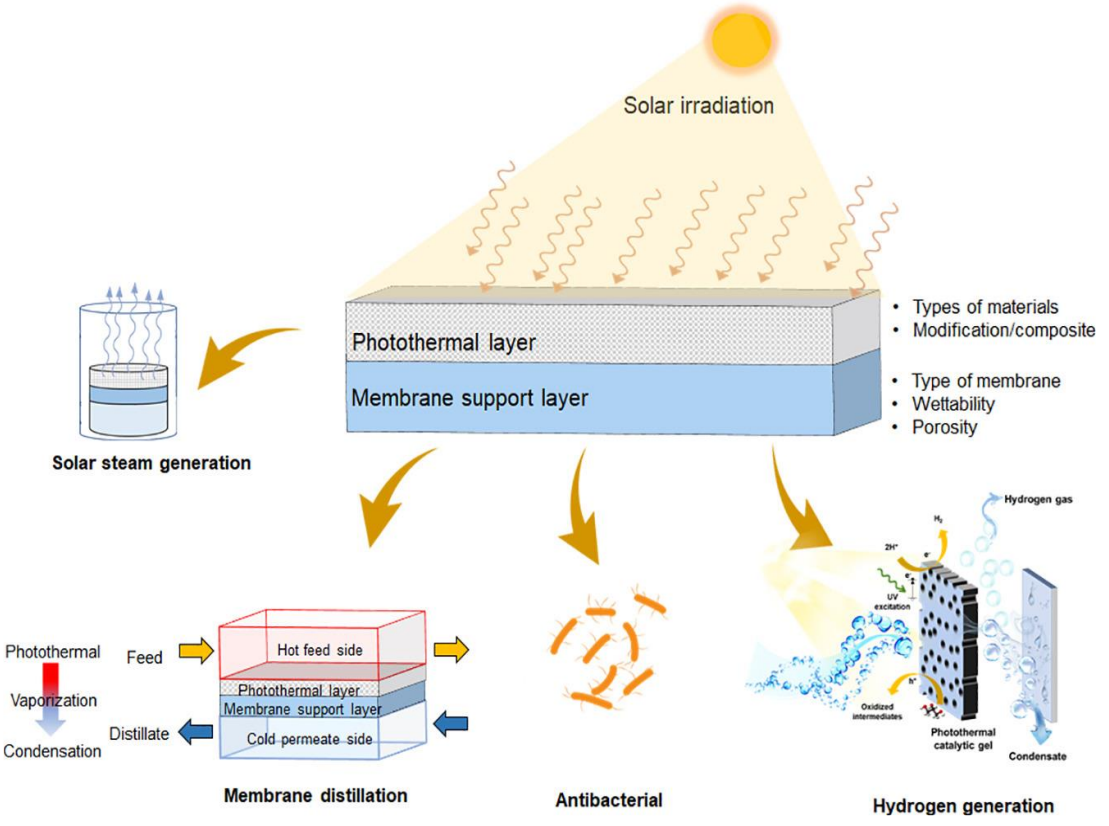

Fig. 3 Schematic diagram of solar-driven water evaporation process. Reproduced with the permission from [22], Copyright Elsevier Desalination.

damage. Existing advanced water evaporation devices raise the bar for the study of interfacial thermal transfer because water evaporation is concentrated on the surface of the membrane. How to localize the heat at the interface is the key to increasing the efficiency of solar-driven water evaporation[20] and therefore, double-layered evaporation structures are proposed.[21] The schematic diagram of advanced solar-driven water evaporation[22] is illustrated in Fig. 3, which includes the photothermal layer and thermally insulating layer. The optimization and design of these two types of layers require an in-depth study of interfacial thermal transport. For a thermally insulating layer, the capacities of water transport and heat isolation are both required, which means that there must be enough channel area to transport water, but with low heat loss. Different surface wettability will lead to different thicknesses of interfacial layers and more attention should be paid to the optimization of the water thickness

Overall, the interfacial liquid structuring and the density depletion depth's role on the interfacial thermal transport should be further studied. New multiscale simulation models and theories need to be developed accurately to capture the physics behind the interfacial thermal transport across the interface, but impossible to include all types of interfaces into one model or theory. The best practice might be setting up multiscale modeling which combines the theory, molecular simulation, and the mesoscale hydrodynamical model to relate the liquid depletion depth with the interfacial thermal transport across the interface. Molecular dynamics simulations can provide critical input parameters such as interfacial thermal conductance, local viscosity, etc. for the next-phase mesoscale simulation to relate the thermal and mass transport across the interface, furthermore, the modeling results/trend can be validated through the experimental measurements on the interfacial thermal transport across the solid/liquid/vapor interface.

Conflict of Interest

There is no conflict of interest.

Supporting Information

Not Applicable.

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