Editorial: Nanoconfined Fluids in Energy Applications

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Editorial on the Research Topic

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Nanoconfined fluids (NCFs) (Sun et al., 2020) exhibit a rich array of physical and chemical phenomena. Formally, a fluid is nanoconfined if it is situated in an environment in which the distance between solid boundaries is of nanometer scale in at least one spatial dimension. NCFs can be confined within a diversity of geometries, including those with cross-sections that are planar [e.g., nanochannels (Neek-Amal et al., 2016)], circular (e.g., nanotubes), or irregular [e.g., various nanopores (Thiruraman et al., 2020; Hassani et al., 2021a; Hassani et al., 2021b)]. NCFs are remarkable for a number of reasons. Chief among these (potentially interconnected) phenomena are surface effects [owing to the high surface-area-to-volume ratios typical of NCF systems (Wang et al., 2019; Wang and Hadjiconstantinou, 2019)], finite-size effects [owing to the comparability of the confining length scale with the fluid internal length scale (Wang and Hadjiconstantinou, 2015)], and even quantum-mechanical effects [owing to the rough comparability of the confining length scale with the thermal de Broglie wavelength (Tocci et al., 2014)]. As a consequence of these effects, NCFs may exhibit many distinctive characteristics in their mass, momentum, and energy transport as compared to their unconfined (bulk) counterparts.

Research on NCFs presents a number of new challenges and opportunities, ranging from experimental design, to simulation methodology, to approaches for uncertainty quantification for material and transport properties of fluids under nanoconfinement (Li and Wang, 2022). Such work is critical for advancing fundamental physics and chemistry; from an engineering perspective, this work can also promote the development of novel energy-related technologies, with applications ranging from energy storage [e.g., supercapacitors (Yoo et al., 2011; Salanne, 2017)], to energy harvesting [e.g., solar evaporation (Liu et al., 2018; Chen et al., 2019) or electricity generation via reverse electrodialysis (Vanoppen et al., 2018; Zhu et al., 2021)], to enhanced oil and gas recovery (Lee et al., 2016), to membrane-based separation processes (Gong et al., 2021). A schematic illustration of energy applications of NCFs is presented in **Figure 1**. In this Research Topic, we aim to present Frontier research in experimental, computational, and theoretical approaches to thermodynamics; mass, momentum, and energy transport; flow physics; and phase behavior of NCFs, especially in energy-related applications. We also aim to discuss and identify research challenges in the field, worthy of the community's broader attention. The main topics of interest in this Research Topic include 1) reviews on recent developments in the field of NCFs, 2) novel experimental and theoretical investigations of NCFs, 3) novel computational studies of NCFs, and 4) NCFs in energy-related applications. In this Research Topic, four high-quality papers were accepted for publication, which we briefly summarize below.

Cui et al. study diffusion of nanoconfined fluids as motivated by problems of shale gas production. In particular, the authors investigate the diffusivity of high-temperature and high-pressure CH_4 gas

FIGURE 1 | Schematic illustration of nanoconfined fluids in energy applications. Inserted figures are adapted from references (Yoo et al., 2011; Lee et al., 2016; Liu et al., 2018; Gong et al., 2021; Zhu et al., 2021).
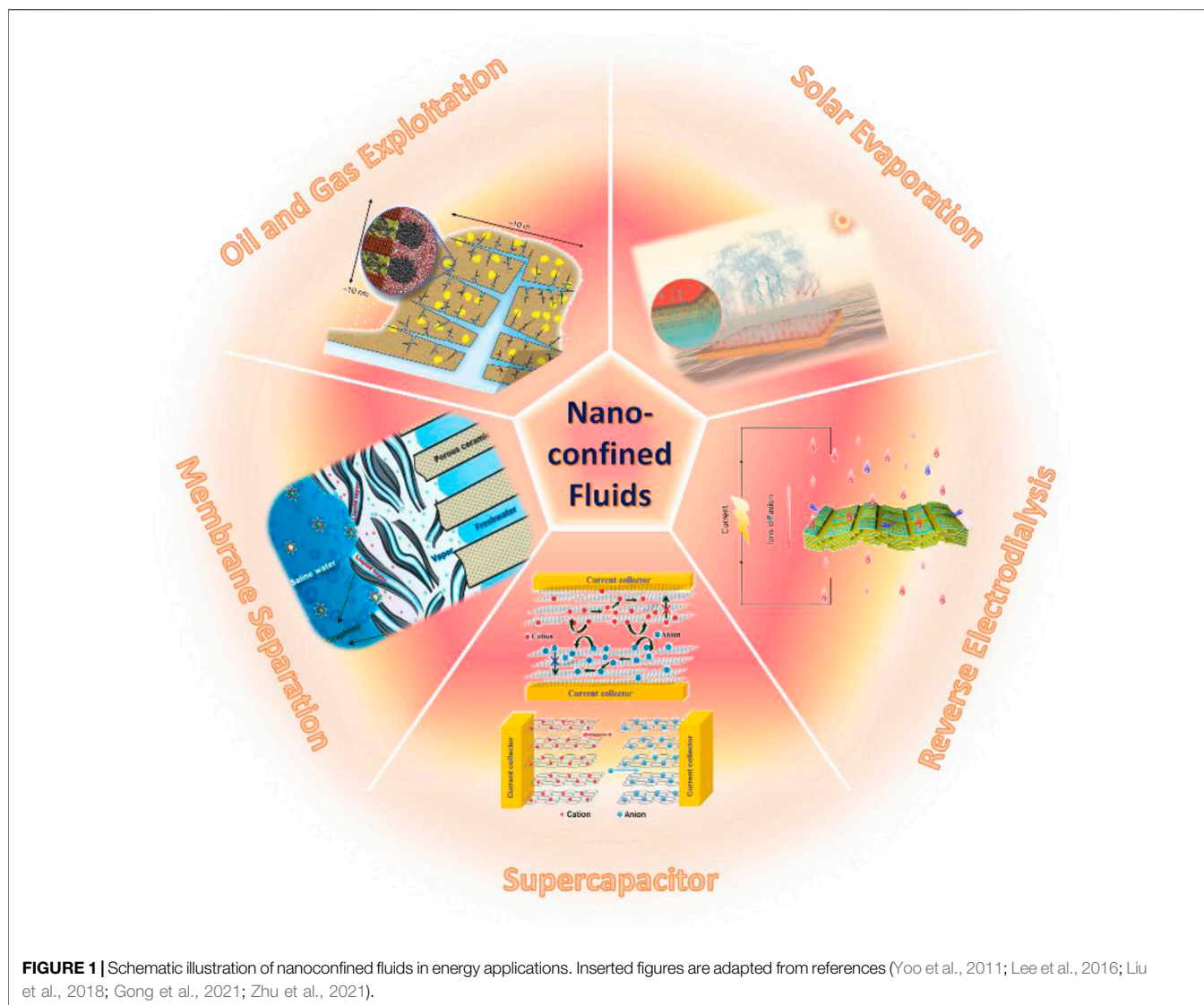
in silica nanochannels by employing molecular-dynamics simulations. Their results show that the diffusivity is clearly anisotropic, owing to restricted motion of fluid molecules near solid walls. Furthermore, their work reveals the dependence of the diffusivity on the channel height and wall potential interaction.

Zhou et al. make a contribution to the fundamental theory of nanoconfined fluids by studying the specific heat capacity of water in graphene nanochannels. They find a commensurability effect within the specific heat capacity data as channel height decreases to 1.7 nm. The anomalous heat capacity of nanoconfined water (as compared to bulk water) originates from the combination of configurational features (as assessed via density distributions and hydrogen bonds) and vibrational features (as assessed via the vibrational density of states). Specific heat capacity is an important thermophysical property related the heat transfer performance of fluids, and thus this work has significance for thermal energy-related applications of nanoconfined fluids.

Yu et al. study nanoconfined fluids in the context of oil production from reservoirs with a matrix permeability of 68.1 mD and an average pore throat radius of 60 nm. They carry out hydrocarbon gas gravity drainage experiments in two dimensions to investigate the influence of reservoir heterogeneity on the gas-oil interface and sweep characteristics of injected gas. In their experiments, they directly observe the miscible zone of crude oil and hydrocarbon gas, and find that the interlayer has a shielding influence that can destabilize the gas-oil interface and miscible zone.

Sun et al. report on membrane separation with two-dimensional nanoporous materials and study the transport of confined gas in nanopores. They investigate a graphene-hexagonal boron nitride bilayer nanopore to realize high-permeance molecular sieving by virtue of quasi-unidirectional molecular transport through nanopores. The quasi-unidirectional molecular transport results from the discrepancy in the gas adsorption abilities on the two sides of bilayer nanopores. The bilayer pore in their work exhibits 3.7 times higher selectivity of CO_2/CH_4 as

compared to the single-layer graphene nanopore of the same size.

In summary, this Research Topic highlights the promising prospects of nanoconfined fluids in energy applications, showcases several areas of exciting current research, and also highlights several open questions in this field. We sincerely hope that more researchers will invest effort in the study of nanoconfined fluids, from basic theory to application, and especially in the context of energy applications.

AUTHOR CONTRIBUTIONS

CS organized the writing of this editorial note and CS, MN-A, GW, and ZZ jointly wrote and edited the final text.

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