Water-methanol mixture segregation and separation under confinement

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Water pollution and renewable energy sources are a matter of broad concern, both environmental challenges for our society. For its applications in the chemical and pharmaceutical industry, production of synthetic fibers and plastic, and as a fuel additive, methanol attracts interest for how to model its properties when mixed with water. Here, we consider a minimalistic model for a water-methanol mixture confined between two parallel graphene nanosheets and analyze the diffusion coefficient of each component as the slit-pore's width δ increases. We find that layering in the hydrophobic pore induces segregation between the two components. The methanol apolar moiety segregates near the pore walls, while water populates more in the central layer away from the hydrophobic walls. Furthermore, both liquids have a diffusion coefficient that changes non-monotonically with δ, with water always diffusing faster than methanol. Changes in the pore width affect the two mixture components in different amounts, suggesting the possibility of an efficient method for methanol-water separation based on a physical procedure.