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ENGINEERING GRAPHENE BY DEFECT DESIGN FOR WATER FILTRATION

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ABSTRACT

While being one-carbon-atom thick, pristine graphene is 200 times stronger than steel. This makes graphene an incredibly multifunctional material with wide applications in composites, energy, and environments. However, producing high-quality graphene is still a challenge, since manufacturing inevitably induces vacancy defects on its surface. While these defects may be deleterious, they also offer tremendous ways to tune the mechanical properties of graphene sheets. Hence, the first objective of this study is to probe the fracture responses of graphene by varying defect properties like defect ratio, shapes, locations, and orientation. To do this, a pristine graphene sheet was first generated for atomistic modelling, and then, a series of defects were created using an in-house developed script. Afterwards, tensile stretch simulations were performed on the graphene sheet, using molecular dynamics techniques. Consistent with literature results, with an increase in vacancy defects, the fracture strength is significantly decreased. In contrast, its fracture strain exhibits a non-monotonic trend, where the initial decrement is followed by increments at large defect ratios. Furthermore, defects with the same size/shape but different orientations were found to result in distinct fracture stresses and strains of graphene sheets. To explore applications of defected graphene, we then functionalized defects and carried out filtration studies.

Filtration is one type of desalination techniques, where water fluxes are driven by pressure gradients to pass through membranes that repel salt species. Graphene with functionalized nanopores attracts great attentions as filtration membranes, given their robust stability, high water flux, and excellent selectivity. Here, we focused on the effects of hydrogenated and hydroxylated groups on the permeability and selectivity of graphene during seawater desalination. Molecular dynamics techniques were again employed as major tools. For all simulations, numbers of salt ions and water molecules, system volumes, and operation temperatures were kept constant, while the applied driving pressures were varied from 300 MPa to 3000 MPa. It was found that with hydrogenated functionalization, graphene membranes of multiple pores have a higher water permeability compared to those with a single pore, resulting from the multiple pathways water molecules can travel through. Additionally, increasing the applied pressure also resulted in higher water permeability, but meanwhile decreased salt rejections. To maintain salt rejections, graphene membranes with hydroxylated pores as well hybrid functionals were further studied to provide detailed comparisons. The results from our work here can help to design functionalized graphene to achieve optimal desalination.