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ABSTRACT

2D Fullerene Membranes for Gas and Water Transport

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It is extremely challenging to create long-range-ordered sub-nanometer pores in carbon materials. Recent breakthroughs in synthesis of covalently linked fullerene networks in gram scales provide a great opportunity to realize 2D and 3D ordered sub-nanometer pores at the interstices among linked C60 units. Here we show from both first principles and molecular dynamics simulations that the square-latticed monolayer fullerene membranes based on the experimental quasi-tetragonal phase of the fullerene 2D network possess the pore size, shape, and geometry promising for gas separations and water transport. Our simulation results suggest that there is a great potential in using covalently-linked-fullerene membranes for separations.