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Predicting hydrogen and methane adsorption in carbon nanopores for energy storage[1] YUNGOK IHM, University of Tennessee, JAMES MORRIS, VALENTINO COOPER, Oak Ridge National Lab, MORRIS LAB, U. TENNESSEE COLLABORATION, ADVANCED MATERIAL GROUP, ORNL COLLABORATION — There are increasing demands for alternate fuels for transportation, which requires safe, high energy density, lightweight storage materials. Experimental measurements and theoretical predictions show relatively low hydrogen storage capacities in various porous materials, limiting hydrogen as a viable alternative for automobiles. In this work, we use a continuum model based on van der Waals density functional (vdW-DF) calculations to elucidate the role that long-range interactions play in the hydrogen adsorption properties of model slit nanopores in carbon. The proper treatment of long-range interactions gives an optimal pore size for hydrogen storage of 8-9 Å (larger than previously predicted). Remarkably, we find a peak hydrogen density close to that of liquid H_2 at ambient temperatures, in agreement with recent experimental results on pore-size dependent adsorption in nanoporous carbon. We then show that such nanopores would be better suited to storing methane, possibly providing an alternative to fill the gap between the capacity required by DOE goals and that attainable with current hydrogen storage technology.

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