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First-principles study of methane adsorption on defective graphitic nanostructures BRANDON WOOD, Theoretical Sciences Unit, JNCASR, Bangalore, India, DEBOSRUTI DUTTA, GANAPATHY AYAPPA, Department of Chemical Engineering, Indian Institute of Science, Bangalore, India, SHOBHANA NARASIMHAN, Theoretical Sciences Unit, JNCASR, Bangalore, India — Efficient storage of methane represents a significant challenge to large-scale implementation of natural gas-based consumer transportation. Activated carbons and related carbon-based nanoporous structures have garnered tremendous interest as storage media due to their unusually high absorptive capacities. However, systematic improvement of these materials relies on a fundamental understanding of the physical and chemical processes involved. We present here extensive energetic calculations of methane adsorption in model carbonaceous systems using density-functional techniques. As exact microstructures of activated carbons are difficult to obtain, we have attempted to isolate likely model nanostructures and defects, including surfaces, edges, point defects, and chemical functionalization. For each of these cases, we analyze changes in the structural, magnetic, and electronic properties upon adsorption. The defect structures exhibiting strongest methane adsorption are isolated, and the relevant mechanisms dominant in binding are identified. The impact of our results in terms of increasing methane absorptive capacity in activated carbons is discussed.

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