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**Ab initio study of H2 adsorption in graphitic BC2N** YI ZHANG, Department of Physics, University of Nevada, Las Vegas, HONG SUN, Department of Physics, Shanghai Jiao Tong University, China, CHANGFENG CHEN, Department of Physics, University of Nevada, Las Vegas — We report results of first-frinciples density functional and quantum Monte Carlo (QMC) calculations on the H2 adsorption in graphitic BC2N. The binding energy and kinetics of H2 at various adsorption sites and coverages are systematically examined. The obtained results provide insights into the mechanism and capacity of hydrogen storage in graphitic BC2N.

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