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Modeling hydrogen storage in boron-substituted graphene decorated with potassium metal atoms

Andrey Tokarev[1], Alexander V. Avdeenkov[2,3,4], Henrietta Langmi[5] and Dmitri G. Bessarabov[1,*,†]

[1]DST Hydrogen Infrastructure Center of Competence (HySA Infrastructure), Faculty of Engineering, North-West University, Private
Bag X6001, Potchefstroom, 2520, South Africa
[2]SSC Institute of Physics and Power Engineering, Obninsk, Russia
[3]National Institute for Theoretical Physics (NITheP), Stellenbosch and Institute of Theoretical Physics, University of Stellenbosch,
Stellenbosch, 7600, South Africa
[4]Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Leninskie Gory 1(2), GSP-1, 119234 Moscow, Russia
[5]HySA Infrastructure Centre of Competence, Materials Science and Manufacturing, Council for Scientific and Industrial Research
(CSIR), PO Box 395, Pretoria, 0001, South Africa

Abstract

Boron-substituted graphene decorated with potassium metal atoms was considered as a novel material for hydrogen storage. Density functional theory calculations were used to model key properties of the material, such as geometry, hydrogen packing, and hydrogen adsorption energy. We found that the new material has extremely high hydrogen storage capacity: 22.5wt%. It is explained by high-density packing of hydrogen molecules into hydrogen layers with specific geometry. In turn, such geometry is determined by the composition and topology of the material.