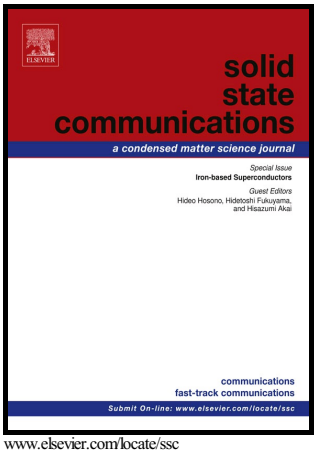

www.elsevier.com/locate/ssc

Intrinsic half metallicity in lithium terminated zigzag graphene nanoribbons

Neha Tyagi, Neeraj K. Jaiswal, Varun Sharma, Kamal K. Jha, Pankaj Srivastava

PII: S0038-1098(16)30329-5
DOI: http://dx.doi.org/10.1016/j.ssc.2016.11.022
Reference: SSC13087

To appear in: *Solid State Communications*

Received date: 31 March 2016
Revised date: 27 September 2016
Accepted date: 25 November 2016

Cite this article as: Neha Tyagi, Neeraj K. Jaiswal, Varun Sharma, Kamal K. Jha and Pankaj Srivastava, Intrinsic half metallicity in lithium terminated zigzag graphene nanoribbons, *Solid State Communications* http://dx.doi.org/10.1016/j.ssc.2016.11.022

Intrinsic half metallicity in lithium terminated zigzag graphene nanoribbons

Neha Tyagi[1*], Neeraj K. Jaiswal[2], Varun Sharma[3], Kamal K. Jha[4], Pankaj Srivastava[3]

[1]Department of Applied Physics, Delhi Technological University, Delhi-110042, India
[2]Discipline of Physics, Indian Institute of Information Technology, Design & Manufacturing, Jabalpur, Dumna Airport Road, Jabalpur-482005, India
[3]Nanomaterials Research Group, ABV-Indian Institute of Information Technology & Management, Gwalior-474015, India
[4]Indian Institute of Information Technology, Vadodara-382028, India
[*]Corresponding author: nehatyagi@dtu.ac.in

Abstract

Half-metallic materials are the prime requisite for future spintronic devices. In present work, the possibility of half-metallic characteristic has been investigated in Li terminated zigzag graphene nanoribbons (ZGNR) using density functional theory. Two different configurations: (i) both edges Li termination (Li-both edges) and (ii) one edge Li termination (Li-one edge), have been examined in the present study. The calculated binding energy (ranging from -3.19 eV to -4.96 eV) confirms that both the considered configurations are energetically viable to obtain. All the considered structures settled in antiferromagnetic ground state which is more stable than that of spin compensated state. Further, it is revealed that upto 100% spin polarization can be achieved (without application of any external electric field) in ZGNR with Li-one edge. Moreover, the observed half-metallicity is found to be independent of the ribbon width and therefore pledges for applications in novel spin filtering devices.

Keywords

A. Graphene nanoribbon; A. lithium; D. binding energy; D. half-metal; D. spintronic