Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Material for

Exploring high-energy and mechanical robust anode materials based on doped graphene in lithium-ion battery: A first-principle study

Cheng Chang [a], Sha Yin [a] and Jun Xu [b, c*]

[a] Department of Automotive Engineering, School of Transportation Science and Engineering, Beihang University, Beijing, 100191, China

[b] Department of Mechanical Engineering and Engineering Science, The University of North Carolina at Charlotte, Charlotte, NC 28223, USA

[c] Vehicle Energy & Safety Laboratory (VESL), North Carolina Motorsports and Automotive Research Center, The University of North Carolina at Charlotte, NC 28223, USA

This Supplementary Information Material Includes

- The computation details of uniaxial and biaxial tensile process
- Figure S1 and figure captions

When performing uniaxial tension calculation of the doped graphene, the strain is put on the zigzag/armchair direction by changing the lattice length step by step. Herein, it should be paid attention that the tensile stress in the zigzag (armchair) direction will lead to the contraction in the armchair (zigzag) direction for the graphene. Therefore, in each step, 5% strain is loaded in the tensile direction and the lattice length in the direction perpendicular to the tensile direction should be relaxed in the calculations. While during the biaxial tension, the strain is put on the zigzag and armchair direction simultaneously.

For the 2-D materials, the stress is calculated based on the thickness of the materials. In this paper, the nominal thickness is considered as 0.34 nm, consistent with the previous study[1]. And thus the calculated stress value obtained from VASP should be divided by the lattice length of the unit cell in the out-off plane direction and then multiply by 0.34 nm, to obtain the real tensile stress.

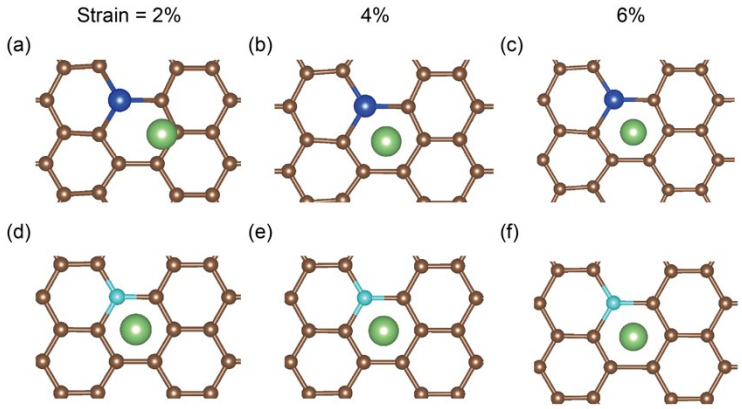

Figure S1. The relaxed structures of Li adsorption on the Si-doped graphene anode with (a) 2%, (b) 4% and (c) 6% biaxial tensile strain. For comparison, the relaxed structures are shown for the B-doped graphene with (d) 2%, (e) 4% and (f) 6% stain, respectively. Brown, cyan, blue and green ball stand for carbon, boron, silicon and lithium atom.

Reference

1 C. Lee, X. Wei, J. W. Kysar and J. Hone, *Science,* 2008, **321**, 385-388.