Thematic Section: Quantum-Chemical Research. **Full Paper**
Subsection: Electrochemistry. *Reference Object Identifier* – ROI: jbc-02/18-53-1-71
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
The article is published based on the materials of the 2nd stage of the Mini-Symposium "Butlerov Heritage – 17-18" (Kazan)
Submitted on January 16, 2018.

Quantum-mechanical calculation of characteristics of the silicene anode for Na-ion batteries

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Keywords: density functional theory, silicene, sodium.

Abstract

As production and consumer demand for electric vehicles are gaining momentum, lithium is becoming a largely deficit metal, therefore, even more expensive. Na-ion batteries are promising candidates for replacing lithium-ion batteries in large-scale applications because of the advantages in natural abundance and the cost of Na. Sodium batteries have a significantly longer service life than lithium batteries and are more stable. In particular, it is possible to expose the sodium-ion battery to a deep discharge, without significantly damaging it. The sodium electrochemical device, in contrast to lithium, is not a fire hazard. The transition from lithium-ion to sodium batteries will lead to an increase in the power of electrochemical current sources and the speed of their charging. Sodium-ion cells can provide a higher charge and discharge current, which is a clear advantage for use in electric vehicles. Silicene has great potential for use as an anode in both lithium-ion batteries and sodium-ion current sources, but it still has not received attention in connection with ionic batteries. Based on the first principles of the density functional theory, the interaction of Na and Li atoms with an autonomous silicene has been studied. Such calculations allow one to compare the behavior of Na or Li ions on silicon films. First, we determined the most stable adsorption sites and their corresponding binding energies for a single Na or Li adatom on the membranes under consideration. Then we gradually increase the concentration of these atoms until the saturation of the surfaces is complete. In addition to the adsorption energy, the Si-Na bond lengths for different locations of the adsorbed alkali metal atoms are also calculated. The spectrum of the density of electronic states for each system is calculated. The integration over the energy of this function gives the number of electrons contained in the region attributed to the atom. In the approximation of the generalized gradient, the band structure of the "silicene/Na" system is calculated. The metallic conductivity arises as a result of complete unilateral adsorption of Na atoms on the silicene.

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