Contribution ID: **399** Type: **Oral**

Mobility of alkali metal atoms in graphene systems with geometric distortions.

Wednesday, 17 April 2019 15:30 (15 minutes)

One of the limiting factors of the charge/discharge rate of lithium-ion batteries and related systems is the low mobility of alkali metal atoms in the anode material. Graphene-based anode materials can improve this and a number of other characteristics. The mobility of atoms in graphene or other intercalates is determined by a number of characteristics associated with lattice vibrations. In the case of highly disordered graphene, small low-layered structures act as a highly deformed matrix material.

This work is dedicated to a theoretical study of the influence of geometry distortion on the mobility of alkali metal atoms in graphene structures. The molecular dynamics simulations have been used to determine the diffusion characteristics of lithium and sodium for a number of single and bilayer structures with different geometric constraints. Significant changes in lattice vibration modes were observed, depending on the nature of the structure constraint. In the case of bilayer structures, this led to a significant isotropy of alkali atoms mobility. This result may be useful for developing advanced batteries and related systems.
The work was financially supported by the Russian Science Foundation (grant №17-73-10226).

Primary author: Mr YAMALETDINOV, Ruslan (NIIC SB RAS)

Presenter: Mr YAMALETDINOV, Ruslan (NIIC SB RAS)

Session Classification: Condensed Matter Physics

Track Classification: Condensed Matter Physics