



573rd ASRC Seminar

Date: 11:00 ~ 12:00, 27 October


Location: Meeting room 302, ASRC Building

Speaker: Dr. Zakhar Popov
(Kirensky Institute of Physics, Russia)

Title: Theoretical investigation of materials
for lithium sorption

Different phases of Li_xSi were investigated by using USPEX code. The energy of the sorption and diffusion of lithium atoms on silicon surface in the process of their transport into nearsurface layers, as well as inside crystalline silicon, at various lithium concentrations have been investigated within the density functional theory.

Calculation of the coefficient of diffusion of lithium into crystalline and amorphous silicon had been performed by using the method based on the calculation of the statistical distribution of potential barriers for the motion of an admixture atom between minima depending on the position of neighboring atoms.



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