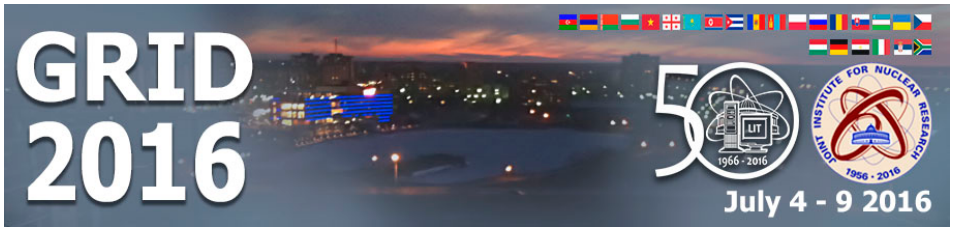

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Formation and stability of structural defects in the crystaline structure of lead dioxide: a DFT study

Monday, 4 July 2016 17:30 (1 hour)

The mechanism of conductibility for lead dioxide - which is the main component of the psoitive electrode of the lead-acid batteries - was elucidated only recently. The DFT calculations as well as experimntal data indicated that a concentration of 1 to 2 percent of deffects in the crystal structure of lead dioxide may result in a signifficant change of the conductibility - which in particular proves to be essential for the functionong of the lead-acid battery.
The aim of our investigation is to determine the energy barrier associated to formation of these defects as well as the geometric parameters characterizing them. To this end we used DFT calculations to point out the value of energy barriers existing between different structures of lead dioxide (i.e. ideal structure as well as structures including defects). We present different structures, the value of energy barriers and the paths connecting the ideal to defect structures.

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