Streszczenie rozprawy doktorskiej mgr Grzegorza Kasprzaka zatytułowanej „Stabilność i degradacja dwuwymiarowych materiałów anodowych na bazie modyfikowanego grafenu"

Two-dimensional (2D) materials are a promising platform for applications in ion battery technology due to their unique physical and chemical properties. In this doctoral thesis, entitled „Stability and degradation of two-dimensional anode materials based on modified graphene", the destruction processes and self-regeneration mechanisms of 2D materials are investigated using ab-initio methods with density functional theory (DFT) and molecular dynamics (AIMD). The work focuses on the analysis of electronic and structural properties and on the exploration of functional parameters of electrode materials, which can significantly affect the performance and lifetime of batteries. In this work, I also focus on the use of other than classical lithium ions, i.e. magnesium and sodium ions. Due to their abundance in the Earth's crust, these elements are much more easily available, but due to their much higher atomic masses, they bring new challenges that must be met by anode materials of high-performance and low-cost ion batteries.

The first part of the thesis presents the motivation and research goal, explaining why two-dimensional materials are crucial for future energy storage technologies. Then, different types of batteries are described, with special emphasis on lithium-ion batteries, which currently dominate the market due to their excellent performance parameters. The next part of the thesis discusses structural defects occurring in two-dimensional materials, which are crucial for understanding the mechanisms of electrode destruction. It describes the main types of defects relevant for materials with reduced dimensionality and typical degradation mechanisms that affect the performance and lifetime of these materials and, consequently, the batteries themselves.

The methodology chapter describes in detail the applied research techniques: molecular orbital theory, electron density functional method, and molecular dynamics from the first principles. These advanced methods allow precise modeling of processes at the atomic level, which is necessary to understand the behavior of materials under conditions as close as possible to the real operating conditions of batteries.

In the main part of this work, a series of two-dimensional materials such as B_2C, C_3N, C_3B, BC_7, NC_7, N_3C_5 and B_3C_5 were analyzed. The B_2C monolayer was investigated as anode material for magnesium batteries, showing a high theoretical charge storage capacity of 3187.55 mAh/g while retaining metallic properties after Mg ion adsorption, making it a promising anode material. AIMD simulations confirmed the stability of the B_2C structure during the charge and discharge process. The C_3N monolayer showed a transition from a semiconductor to a metallic state after Li/Na adsorption and a theoretical capacity of 267.82 mAh/g, indicating its potential as anode material for

Li/Na-ion batteries.

Studies on intercalated C_3N have shown a significant increase in the interlayer distance upon intercalation of lithium and sodium ions, which may ultimately limit the application of sodium, but does not exclude its use under appropriate conditions. In a comparison of C_3B, C_3N and graphene materials, it has been shown that C_3B after Li/Na intercalation maintains stability, while C_3N does not return to the ground state upon this process, making it a less suitable anode material compared to C_3B and graphene.

The bilayer BC_7 material showed a significant swelling effect after intercalation with Na and Mg ions, which limits its application to Na/Mg-ion batteries. However, after the simulated lithium intercalation process, BC_7 shows a high theoretical capacity of 423.69 mAh/g while offering low barriers to ion diffusion on its surface. This parameter may make it a promising anode material. Studies on the NC_7 material have shown its high thermal stability and its metallic character in mono- and bilayer forms. At the same time, NC_7 after intercalation with Li ions shows a high theoretical capacity of 683.14 mAh/g, but large volume changes after intercalation with Na and Mg eliminate this material as a candidate for anode for batteries in which Na or Mg ions are used instead of lithium. New materials, such as B_3C_5 and N_3C_5, were also investigated for their potential use as anode materials. B_3C_5 exhibits excellent electrical conductivity, relatively low diffusion barrier for Li ions (0.27 eV) and high theoretical capacity of 579.57 mAh/g, which suggests its high suitability as an anode material. N_3C_5 loses stability after intercalation with Li ions, which excludes it from further analysis. The dissertation ends with a summary of the most important conclusions and indication of potential directions for further research, with particular emphasis on practical applications of the studied materials in the production of modern ion batteries and their self-regeneration ability, which can significantly extend their lifetime and improve their efficiency.