THE BALTIC ASSEMBLY PRIZE IN SCIENCE 2020: THEORETICAL PREDICTIONS OF NEW MATERIALS FOR ENERGY STORAGE AND HARVESTING

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TOWARDS A PRACTICAL RECHARGEABLE 5 VOLT LI ION BATTERY

One of the three Nobel Prize winners in chemistry in 2019, J. Goodenough (USA), in 1980, discovered the cathode material for 4 Volt batteries $LiCoO_2$. Nowadays, consumer electronics widely use lithium-ion batteries containing $LiCoO_2$, for example, in laptop computers, cellular telephones, electric vehicles as well as airplanes and even cosmic technologies. One frequently discussed direction to improve the performance of 4 Volt batteries is the development of a family of 5 Volt cathode materials. We were the first in the world to theoretically predict that also a 5 Volt battery is possible [1]. Namely, by means of a Full Potential Linearized Augmented Plane Wave (FP-LAPW) calculations for $Li_2CoMn_3O_8$ battery cathode material we got the average battery voltage for this material around 5 Volt [1].

THEORY EXPLAINING SYSTEMATIC TRENDS IN PROPERTY CHANGES FOR ABO_3 PEROVSKITE SURFACES

We performed *ab initio* calculations for eight technologically most important ABO_3 perovskite neutral (001) as well as very complex, polar and charged (011) surfaces [2–7]. As a result of our calculations, we developed a theory, which describes systematic trends in property changes for ABO3 perovskite (001) as well as (011) surfaces [2–7]. For example, based on our calculations, we discovered, that surface energies for both AO and BO_2-terminated ABO_3 perovskite (001) surfaces are almost equal. Just opposite for polar (011) and especially (111) surfaces, their energies for different terminations are completely different [2–7].

ENHANCEMENT OF THE PHOTOELECTRIC CONVERSION EFFICIENCY BY GRAPHENE OF A DYE SENSITISED SOLAR CELL

Solar energy, as an alternative energy source, has attracted more and more attention in the past few decades [8]. The dye-sensitised solar cell (DSSC) has been a hot topic due to its low cost and relatively high photoelectric conversion efficiency since the first device was reported in 1991. The main goal of our work was to clearly answer the question from a theoretical perspective: how does graphene enhance the photoelectric conversion efficiency in the semiconducting layer of a dye sensitised solar cell? Several arrangements of the graphene layer between the dye molecule and the TiO_2 (101) surface are carefully studied and discussed. Our theoretical investigation shows that graphene can speed up the electron injection from the dye molecules to the semiconductor layer [8].

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THE EFFECTS OF IMPURITIES IN 4,12,2-GRAPHYNE

The effects of boron (B) and nitrogen (N) substitutions in 4,12,2-graphyne on its geometric structure and mechanical as well as electronic properties have been systematically investigated with the aid of DFT [9]. The trend in the elastic properties of the substituted systems is determined by the doping positions and the type of the dopants. In particular, we discovered an obvious in-plane piezoelectricity induced by foreign atom substitutions owing to the deformation of the pristine square symmetry [9].

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