Uptake of Carbon Dioxide by Carbon Spiroids

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Spiral carbon nanoparticles (spiroids) are relatively new types of nanoclusters [1-4] with the unique geometry that might be very prospective for possible applications ranging from hydrogen storage, transport and related energy applications, drug delivery for biochemistry and medicine, up to new types of nanocapacitors [4]. Further understanding of the carbon dioxide adsorption mechanisms might be useful for the novel technologies meant to deal with the global warming process through the reduction of the CO_2 atmospheric concentration by sequestration. Therefore, the adsorption of the CO_2 to various carbon compounds has been earlier research topic. In particular, we have previously studied adsorption mechanisms of carbon dioxide to graphene layers [5].

In the present studies, we use *ab initio* Car-Parrinello molecular dynamics [6] method in the framework of the density functional theory (DFT) with the energy functional containing van der Waals (vdW) correction to analyze the capability of carbon dioxide to be adsorbed by spiroids in a comparison with carbon spheroids. The goal of the study is to demonstrate whether the maximum concentration of absorbed carbon dioxide might be obviously achieved for the case of carbon spiroidal particle in comparison with spheroidal one, containing the same number of atoms. The stability and dynamics of the spiral carbon nanoonion- adsorbed carbon dioxide is studied in the temperature range 4.2 to 2000 K.

This work has been supported by the SHALESEQ project within the Polish-Norwegian Research Program (EEA Grant PL12-0109)

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