Annual meeting of the COST Action: *Computational materials sciences for efficient water splitting with nanocrystals from abundant elements (CA18234)*

"Computational water splitting, where we are now and where to go?

February 14-15, 2022, on-line event

Stability of the hematite supported oxide nanoclusters from MD simulations

Bartłomiej M. Szyja[1], *Wiktor Żuczkowski*[1], *Tomasz Dymkowski*[1], *Wojciech Kołodziekczyk*[2], *Glake Hill*[2]

[1]Advanced Materials Engioneering and Modeling Group, Faculty of Chemistry, Wrocław University of Science and Technology, Wrocław, Poland

[2]Interdisciplinary Center for Nanotoxixity, Jackson State University Mississippi, Jackson MS, USA

b.m.szyja@pwr.edu.pl

In this work we present the result of the MD simulations on the stability of the TiO_2 nanoclusters supported on the hematite surface. The clusters have been selected basing on their structures cotaining 2, 3 or 4 Ti atoms. The initial configuration of the slusters have been determined basing on the in-house developed algorithm based on the Monte Carlo assumptions. In particular, the clusters have been randomly rotated and translated within the supercell containing the hematite (110) surface. Then the contacts have been evaluated and sreened with respect to the optimal distances between the nanoclusters and the surface. Subsequently, the energy of the system was evaluated using a very coarse DFT simulations in order to provide the most optimal geometries and remove the most unstable from the set. This led to the collection of 20 initial geometries for each of the investigated nanoclusters.

Each of the nanoclusters have been then simulated with the MD approach on the high level DFT method. The results allowed us to determine the most stable configurations of the nanoclusters. The energy profiles were able to provide the data on the reconstruction of the nanoclusters upon the interactions with the hematite furfaces. We have determined the following possible mechanisms to be involved: (1) the elekctrostatic interactions leading to the change of the orientation of the nanocluster; (2) change of the bond order of the Ti-O bond; (3) the cleavage of the oxygen bridge between two Ti atoms.

The next step is the determination of the role of the nanocluster-surface interactions on the band structure of the most stable system configuration.