DELIVERABLE REPORT

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SONAR

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1 Introduction

This deliverable describes the contents of a database of calculated parameters that will be used for the mesoscale kinetic Monte Carlo simulations in WP3.

2 Description of the database

The goal of task 2.3 is to develop computational protocols for electronic structure calculations needed for the parametrization of mesoscale models developed by LRCS in WP3. The methods are described in detail in the WP2 technical progress report due M18.

The databases containing the computed parameters are accessible to all project partners on the SONAR cloud under SONAR-Share/WP-3/Data/

The file ads_en_graphene_flake_GFN_sol_geom.csv contains the adsorption energies of selected molecules on the basal plane of a finite graphene flake. The column separator character is ‘,’. The columns are:

mol: name or acronym of the molecule, specifying also the pH if relevant and the charge or oxidation state (o = oxidized, r2 = reduced with 2 electrons)

E_{ads}(GFN-xTB) [eV]: adsorption energy computed with the GFN-xTB semiempirical method.

E_{ads}(DFT at GFN-xTB geom) [eV]: adsorption energy computed with DFT at the geometries optimized with GFN-xTB.

The file reorg_redox.csv contains the reorganization energies for the redox reactions of selected molecules. The column separator character is ‘,’. The columns are:

id: name or acronym of the molecule. The redox reaction is the most relevant one if not specified.

lambda_ox [eV]: reorganization energy of the oxidized form

lambda_red [eV]: reorganization energy of the reduced form

lambda_ave [eV]: average of lambda_ox and lambda_red

3 Conclusion

The databases will be updated when the computational methods are refined and expanded with further molecules if necessary.