DFT data for „Effect of Water on Diffusion Energy Barriers of S_{ad} on Cu(100) and Ag(100) Surfaces“ (rev.)

The archives contain density functional theory (DFT) data for the publication „Falk Wendorff, Chalong Yang, Sönke Buttenschön, Mitja Funk, Olaf M. Magnussen and Eckhard Pehlke, Effect of Water on Diffusion Energy Barriers of S_{ad} on Cu(100) and Ag(100) Surfaces“ (DOI: `https://doi.org/10.1021/acselectrochem.5c00414`).

For details see the original publication. Data have been created using programs from the software package „Quantum ESPRESSO“ [1,2] and „Environ“ [3]. Pseudopotentials from repositories have been used. Detailed references for the pseudopotentials and repositories are listed in the Supporting Information of the original publication. Initial water structures have been created using the Water Structure Creator software by A. C. Dávila López et al. [4]. Data regarding continuum solvation is based on previous work by M. Funk (Master thesis, Kiel, (2024)), please refer to Ref. [5]. Please cite the relevant publications when using the data.

In DFT_simulation_data_Cu100.tar.gz the input files for ionic relaxations with force convergence threshold $10^{-5}\,\mathrm{Ry}/a_0$ have been replaced. The electronic convergence threshold requirement for selfconsistency $10^{-8}\,\mathrm{Ry}$ and the ionic dynamics method ‘damp’ was used to produce the output files. The output files have not been changed.

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), project 504552981. This research was supported in part through high-performance computing resources available at the Kiel University Computing Centre.

[1] P. Giannozzi et al., J. Phys. Condens. Matter 21 395502 (2009).
[2] P. Giannozzi et al., J. Phys. Condens. Matter 29 465901 (2017).
[3] O. Anreussi, I. Dabo, and N. Marzari, J. Chem. Phys.136, 064102 (2012).
[4] A. C. Dávila López et al., J. Chem. Phys. 155 194702 (2021).
[5] F. Wendorff et al., original publication, `https://doi.org/10.1021/acselectrochem.5c00414`.