

Data for: Stress-corrosion cracking sensitization by hydrogen upon oxidation of nickel-base alloys by water - An experiment-guided first-principles study

SND-ID: 2024-41. **Version:** 1. **DOI:** <https://doi.org/10.5878/406j-b839>

Download data

brucite_pressure.ipynb (49.73 KB)

brucite.db (100 KB)

bulk.db (104 KB)

enthalpies_of_formation.ipynb (39.61 KB)

gasphase.db (68 KB)

input_sstructures.ipynb (87.44 KB)

interfaces.db (92 KB)

percentage_errors.ipynb (10.6 KB)

README.md (3.44 KB)

Associated documentation

README.md (3.44 KB)

Download all files

2024-41-1.zip (~558.27 KB)

Citation

Meier de Andrade, A. (2024) Data for: Stress-corrosion cracking sensitization by hydrogen upon oxidation of nickel-base alloys by water - An experiment-guided first-principles study (Version 1) [Data set]. Chalmers University of Technology. Available at: <https://doi.org/10.5878/406j-b839>

Creator/Principal investigator(s)

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Research principal

[Chalmers University of Technology](#) - Chemistry and chemical engineering, Energy and material, Environmental Inorganic Chemistry 2

Principal's reference number

2023-00209

Description

Data material contains (i) the final output of Density Functional Theory calculations stored in Atomic Simulation Environment (ASE) databases and (ii) Python Jupyter notebooks that were used to calculate reactions enthalpy of formation, structural parameters, and percentage errors based on outputs stored in these databases.

Data contains personal data

No

Language

[English](#)

Data format / data structure

[Numeric](#)

[Text](#)

[Interactive resource](#)

[Other](#)

Data collection 1

- Mode of collection: Simulation
- Description of the mode of collection: Data was collected from outputs of atomistic simulations using python scripts employing the Atomic Simulation Environment (ASE) library.

Responsible department/unit

Chemistry and chemical engineering, Energy and material, Environmental Inorganic Chemistry 2

Contributor(s)

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Funding 1

- Funding agency: Swedish Research Council
- Funding agency's reference number: 2023-00209
- Project name on the application: Vätes inverkan på legeringsprestanda: När förvänta sig vad

Funding 2

- Funding agency: Swedish Radiation Safety Authority
- Funding agency's reference number: SSM2021-822
- Project name on the application: Atomistisk modellering av nickelbaslegeringars spänningskorrosion i lättvattenreaktorer

Research area

[Materials chemistry](#) (Standard för svensk indelning av forskningsämnen 2011)

[Inorganic chemistry](#) (Standard för svensk indelning av forskningsämnen 2011)

[Theoretical chemistry](#) (Standard för svensk indelning av forskningsämnen 2011)

[Condensed matter physics](#) (Standard för svensk indelning av forskningsämnen 2011)

[Physical chemistry](#) (Standard för svensk indelning av forskningsämnen 2011)

[Corrosion engineering](#) (Standard för svensk indelning av forskningsämnen 2011)

[Metallurgy and metallic materials](#) (Standard för svensk indelning av forskningsämnen 2011)

Keywords

[Corrosion](#), [Density functional theory](#), [Nickel alloys](#), [Nickel oxides](#)

Accessibility level

Access to data through SND

Data are freely accessible

Use of data

[Things to consider when using data shared through SND](#)

License

[Public Domain Mark 1.0](#)

Versions

Version 1. 2024-04-03

Download metadata

[DataCite](#)

[DDI 2.5](#)

[DDI 3.3](#)

[DCAT-AP-SE 2.0](#)

[JSON-LD](#)

[PDF](#)

[Citation \(CSL\)](#)

[File overview \(CSV\)](#)

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