



## Johannes Voss

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### Bio

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#### BIO

Johannes Voss is Staff Scientist at the SUNCAT Center for Interface Science and Catalysis at SLAC National Accelerator Laboratory. He leads a research team focused on the atomic-level understanding and computational design of systems of relevance for renewable storage and conversion of energy. The team employs data-scientific approaches to improve the predictive power of super computer simulations for chemical reactions with emphasis on heterogeneous catalysis.

#### EDUCATION AND CERTIFICATIONS

- PhD, Technical University of Denmark , Physics (2009)
- MSc, University of Hamburg , Physics (2004)

#### LINKS

- Group Site: <https://web.stanford.edu/group/suncat/vossgroup/>
- SUNCAT Center for Interface Science and Catalysis: <http://suncat.stanford.edu/>
- Personal Site: <https://stanford.edu/~vossj/slac/>

### Publications

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#### PUBLICATIONS

- **Density Functional Tight-Binding Models for Band Structures of Transition-Metal Alloys and Surfaces across the d-Block.** *Journal of chemical theory and computation*  
Balzaretti, F., Voss, J.  
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- **Interpretable Machine Learning Models for Practical Antimonate Electrocatalyst Performance.** *Chemphyschem : a European journal of chemical physics and physical chemistry*  
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- **Factors Affecting the Electron Conductivity in Single Crystal  $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$  and  $\text{Li}_7\text{P}_3\text{S}_{11}$**  *ACS APPLIED ENERGY MATERIALS*  
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- **X-ray free electron laser studies of electron and phonon dynamics of graphene adsorbed on copper** *PHYSICAL REVIEW MATERIALS*  
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- **Data-driven and constrained optimization of semi-local exchange and nonlocal correlation functionals for materials and surface chemistry** *JOURNAL OF COMPUTATIONAL CHEMISTRY*  
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- **Hubbard-corrected oxide formation enthalpies without adjustable parameters** *JOURNAL OF PHYSICS COMMUNICATIONS*  
Voss, J.  
2022; 6 (3)
- **Simulations of x-ray absorption spectra for CO desorbing from Ru(0001) with transition-potential and time-dependent density functional theory approaches** *STRUCTURAL DYNAMICS-US*  
Rodrigues, G. S., Diesen, E., Voss, J., Norman, P., Pettersson, L. M.  
2022; 9 (1): 014101
- **MCML: Combining physical constraints with experimental data for a multi-purpose meta-generalized gradient approximation.** *Journal of computational chemistry*  
Brown, K., Maimaiti, Y., Treppe, K., Bligaard, T., Voss, J.  
2021
- **Ultrafast Adsorbate Excitation Probed with Subpicosecond-Resolution X-Ray Absorption Spectroscopy.** *Physical review letters*  
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- **Theoretical Investigations of the Electrochemical Reduction of CO on Single Metal Atoms Embedded in Graphene** *ACS CENTRAL SCIENCE*  
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- **Li+ Defects in a Solid-State Li Ion Battery: Theoretical Insights with a Li3OCl Electrolyte** *CHEMISTRY OF MATERIALS*  
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