

Steen Lysgaard - DTU Orbit (08/08/2016)

Lysgaard, Steen
stly@dtu.dk

Department of Energy Conversion and Storage - Postdoc

Atomic scale modelling and materials

Theoretical Atomic-scale Physics

Publications:

Accelerated DFT-Based Design of Materials for Ammonia Storage

Jensen, P. B., Bialy, A., Blanchard, D., Lysgaard, S., Reumert, A. K., Quaade, U. J. & Vegge, T. 2015 In : *Chemistry of Materials*. 27, 13, p. 4552–4561 10 p.

Publication: Research - peer-review › Journal article – Annual report year: 2015

A DFT-based genetic algorithm search for AuCu nanoalloy electrocatalysts for CO₂ reduction

Lysgaard, S., Myrdal, J. S. G., Hansen, H. A. & Vegge, T. 2015 In : *Physical Chemistry Chemical Physics*. 17, p. 28270-28276 7 p.

Publication: Research - peer-review › Journal article – Annual report year: 2015

Computational Search for Improved Ammonia Storage Materials

Jensen, P. B., Lysgaard, S., Vegge, T. & Quaade, U. 2014

Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

Designing mixed metal halide amines for ammonia storage using density functional theory and genetic algorithms

Jensen, P. B., Lysgaard, S., Quaade, U. J. & Vegge, T. 2014 In : *Physical Chemistry Chemical Physics*. 16, p. 19732-19740

Publication: Research - peer-review › Journal article – Annual report year: 2014

Designing New Materials for Ammonia Storage Using Density Functional Theory and Genetic Algorithms

Jensen, P. B., Lysgaard, S., Quaade, U. J. & Vegge, T. 2014

Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

Genetic Algorithm Procreation Operators for Alloy Nanoparticle Catalysts

Lysgaard, S., Landis, D. D., Bligaard, T. & Vegge, T. 2014 In : *Topics in Catalysis*. 57, 1-4, p. 33-39

Publication: Research - peer-review › Journal article – Annual report year: 2013

Computational analysis of gas-solid interactions in materials for energy storage and conversion

Lysgaard, S., Vegge, T. & Bligaard, T. 2013 Kgs. Lyngby: Technical University of Denmark. 137 p.

Publication: Research › Ph.D. thesis – Annual report year: 2013

Computational design of catalysts, electrolytes and materials for energy storage

Vegge, T., Howalt, J. G., Lysgaard, S., Myrdal, J. S. G., Bork, N. & Hummelshøj, J. S. 2013 *New and Future Developments in Catalysis: Batteries, Hydrogen Storage and Fuel Cells*. Suib, S. (ed.). Elsevier Science, p. 499-521

Publication: Research - peer-review › Book chapter – Annual report year: 2013

Computational screening of mixed metal halide amines

Jensen, P. B., Lysgaard, S., Quaade, U. & Vegge, T. 2013

Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Computational screening of mixed metal halide amines

Jensen, P. B., Lysgaard, S., Quaade, U. & Vegge, T. 2013 In : *Abstracts of Papers of the American Chemical Society*. 245, 1 p., 122-COMP

Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2013

Surface adsorption in strontium chloride amines

Ammitzbøll, A. L., Lysgaard, S., Klukowska, A., Vegge, T. & Quaade, U. J. 2013 In : Journal of Chemical Physics. 138, 16, p. 164701 6 p.

Publication: Research - peer-review › Journal article – Annual report year: 2013

Computational Screening of Mixed Metal Halide Amines

Jensen, P. B., Lysgaard, S., Quaade, U. & Vegge, T. 2012

Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2012

Genetic Algorithms for Improved Stability of Nanoparticle Catalysts

Lysgaard, S., Bliggard, T. & Vegge, T. 2012

Publication: Research - peer-review › Poster – Annual report year: 2012

Resolving the stability and structure of strontium chloride amines from equilibrium pressures, XRD and DFT

Lysgaard, S., Ammitzbøll, A. L., Johnsen, R., Norby, P., Quaade, U. J. & Vegge, T. 2012 In : International Journal of Hydrogen Energy. 37, 24, p. 18927-18936

Publication: Research - peer-review › Journal article – Annual report year: 2012

Computational analysis of the interaction of water with materials for energy storage

Lysgaard, S. 2010

Publication: Research › Poster – Annual report year: 2010

Computational analysis of the interaction of water with materials for energy storage

Lysgaard, S. 2010

Publication: Research › Poster – Annual report year: 2010

Computational screening and design of complex materials for hydrogen storage and solid electrolytes

Vegge, T., Hummelshøj, J. S., Maronsson, J. B., Myrdal, J. S. G. & Lysgaard, S. 2010 *Book of Abstracts*. American Chemical Society

Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2011

Strontium amines - bulk phases and surface states

Lysgaard, S. 2010

Publication: Research › Poster – Annual report year: 2010

Strontium amines - bulk phases and surface states

Lysgaard, S. 2010

Publication: Research › Poster – Annual report year: 2010

Strontium amines - bulk phases and surface states

Lysgaard, S. 2010

Publication: Research › Poster – Annual report year: 2010

Projects:

Computational analysis of the interaction of water with materials for energy storage

Lysgaard, S., Vegge, T., Bligaard, T., Rossmeisl, J., Hellman, A. & Jónsson, H.

15/09/2009 → 19/03/2013

Project: PhD

Activities:

Theoretical studies of NH₃, H₂O, N₂ and H₂ diffusion in Mg(NH₃)₆Cl₂

Steen Lysgaard (Speaker), 14 Jun 2010 → 15 Jun 2010

Activity: Lecture and oral contribution

***Strontium ammines - bulk phases and surface states**

Steen Lysgaard (Speaker), 8 Nov 2010

Activity: Lecture and oral contribution