List of selected publications for Mie Andersen:

1) Martin Deimel, Karsten Reuter, **Mie Andersen**. *Active site representation in first-principles microkinetic models: Data-enhanced computational screening for improved methanation catalysts*. Submitted.

2) Andrea Auer, **Mie Andersen**, Eva-Maria Wernig, Nicolas G. Hörmann, Nico Buller, Karsten Reuter, Julia Kunze-Liebhäuser. *Self-activation of copper electrodes during CO electro-oxidation in alkaline electrolyte*. Nat. Catal. (in press).

3) Juan Santiago Cingolani, Martin Deimel, Simone Köcher, Christoph Scheurer, Karsten Reuter, **Mie Andersen**. *Interface between graphene and liquid Cu from molecular dynamics simulations*. J. Chem. Phys. (in press).

4) **Mie Andersen**, Juan Santiago Cingolani, Karsten Reuter. *Ab initio thermodynamics of hydrocarbons relevant to graphene growth at solid and liquid Cu surfaces*. J. Phys. Chem. C **123**, 22299 (2019).

5) Albert Bruix, Johannes T. Margraf, **Mie Andersen**, Karsten Reuter. *First-principles-based multiscale modelling of heterogeneous catalysis*. Nat. Catal. **2**, 659 (2019).

6) **Mie Andersen**, Chiara Panosetti, Karsten Reuter. *A Practical Guide to Surface Kinetic Monte Carlo Simulations*. Front. Chem. **7**, 202 (2019).

7) **Mie Andersen**, Sergey Levchenko, Matthias Scheffler, Karsten Reuter. *Beyond scaling relations for the description of catalytic materials*. ACS Catal. **9**, 2752 (2019).

8) **Mie Andersen**, Xiaojuan Yu, Matthias Kick, Yuemin Wang, Christof Wöll, Karsten Reuter. *Infrared reflection–absorption spectroscopy and density functional theory investigations of ultrathin ZnO films formed on Ag (111)*. J. Phys. Chem. C **122**, 4963 (2018).

9) **Mie Andersen**, Craig Plaisance, Karsten Reuter. *Assessment of mean-field microkinetic models for CO methanation on stepped metal surfaces using accelerated kinetic Monte Carlo.* J. Chem. Phys. **147**, 152705 (2017).

10) **Mie Andersen**, Andrew J. Medford, Jens K. Nørskov, Karsten Reuter. *Scaling-Relation-Based Analysis of Bifunctional Catalysis: The Case for Homogeneous Bimetallic Alloys.* ACS Catal. **7**, 3960 (2017).

11) Karsten Reuter, Craig Plaisance, Harald Oberhofer, **Mie Andersen**. *Perspective: On the Active Site Model in Computational Catalyst Screening*. J. Chem. Phys. **146**, 040901 (2017).

12) **Mie Andersen**, Andrew J. Medford, Jens K. Nørskov, Karsten Reuter. *Analyzing the Case for Bifunctional Catalysis.* Ang. Chem. Int. Ed. **55**, 5210 (2016).

13) **Mie Andersen**, Liv Hornekær, Bjørk Hammer. *Understanding intercalation structures formed under graphene on Ir(111).* Phys. Rev. B **90**, 155428 (2014).

14) Richard Balog, **Mie Andersen**, Bjarke Jørgensen, Zeljko Sljivancanin, Bjørk Hammer, Alessandro Baraldi, Rosanna Larziprete, Philip Hofmann, Liv Hornekær, Silvano Lizzit. *Controlling hydrogenation of graphene on Ir(111).* ACS Nano **7**, 3823 (2013).

15) Louis Nilsson, **Mie Andersen**, Richard Balog, Erik Lægsgaard, Philip Hofmann, Flemming Besenbacher, Bjørk Hammer, Ivan Steensgaard, Liv Hornekær. *Graphene coatings: Probing the limits of the one atom thick protection layer*. ACS Nano **6**, 10258 (2012).

16) **Mie Andersen**, Liv Hornekær, Bjørk Hammer. *Graphene on metal surfaces and its hydrogen adsorption: A meta-GGA functional study*. Phys. Rev. B **86**, 085405 (2012).

17) Richard Balog, Bjarke Jørgensen, Louis Nilsson, **Mie Andersen**, Emile Rienks, Marco Bianchi, Mattia Fanetti, Erik Lægsgaard, Alessandro Baraldi, Silvano Lizzit, Zeljko Sljivancanin, Flemming Besenbacher, Bjørk Hammer, Thomas G. Pedersen, Philip Hofmann, Liv Hornekær. *Bandgap opening in graphene induced by patterned hydrogen adsorption*. Nat. Mater. **9**, 315 (2010).