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**Author:** Cao, K.

**Title:** Structure dependence of molecular reactions on surfaces

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# List of publications

**This thesis is based on the following publications**

## Chapter 3

*A molecular beam study of  $D_2$  dissociation on Pt(111): testing SRP-DFT calculations*

Chemical Physics Letters, 2018, 706, pp 680-683

Kun Cao, Richard van Lent, Aart W. Kleyn, and Ludo B. F. Juurlink

## Chapter 4

*Anomalous dependence of the reactivity on the presence of steps: dissociation of  $D_2$  on Cu(211)*

The Journal of Physical Chemistry Letters, 2018, 9(1), pp 170–175

Gernot Fücksel, Kun Cao, Süleyman Er, Egidius W. F. Smeets, Aart W. Kleyn, Ludo B. F. Juurlink, and Geert-Jan Kroes

*The first two authors contributed equally to this paper*

*Hydrogen adsorption and desorption from Cu(111) and Cu(211)*

Physical Chemistry Chemical Physics, 2018, Accepted Manuscript

Kun Cao, Gernot Fücksel, Aart W. Kleyn, and Ludo B.F. Juurlink

*This article is part of the themed collection: “2018 PCCP HOT Articles”*

## Chapter 5

*Structure dependence of HD formation on curved Pt(111) surface*

In preparation

Kun Cao, Aart W. Kleyn, and Ludo B. F. Juurlink

## Chapter 6

*The two faces of step defects in O<sub>2</sub> reaction on Pt*

Nature Chemistry, in preparation

Kun Cao, Mitsunori Kurahashi and Ludo B. F. Juurlink

## Other publications

*Resolving an old problem: how does H<sub>2</sub> dissociate on Pt?*

Science, submitted

Richard van Lent, Sabine V. Auras, Kun Cao, Anton J. Walsh, Michael A. Gleeson and Ludo B. F. Juurlink

# Curriculum Vitae

Kun Cao was born in Zhumadian, a city in Henan province in China in 1986. He obtained his bachelor degree in Tsinghua University in 2008. He obtained his master degree in China Academy of Engineering Physics in 2011. From 2011 to 2014, he worked at China Academy of Engineering Physics as an assistant research fellow. In September 2014, Kun started his PhD research at Leiden University (the Netherlands) in the group “Catalysis and Surface Chemistry” (CASC). The research was carried out under the supervision of Prof. Dr. Marc T. M. Koper, Prof. Dr. Aart W. Kleyn and Dr. Ludo B. F. Juurlink and sponsored by the China Scholarship Council (CSC). The topic of his work was structure dependence of molecular reactions on surfaces. The results are presented in this thesis. Parts of the results have been presented at the following conferences:

- Chemistry As Innovating Science (CHAINS) in Veldhoven, the Netherlands in 2014 (poster)
- International Conference on Molecular Energy Transfer in Complex Systems (ICOMET) in Chengdu, China in 2015 (poster)
- International Conference on Scattering of Atoms and Molecules from Surfaces (SAMS) in Bergen, Norway in 2016 (poster)