# Dissociative chemisorption of methane on Ni(111)

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# List of publications

This thesis is based on the following publications:

- *Towards an understanding of the vibrational mode specificity for dissociative chemisorption of $CH_4$ on Ni(111): a 15 dimensional study*, G. P. Krishnamohan, R. A. Olsen, Á. Valdés, and G. J. Kroes, Phys. Chem. Chem. Phys., **12**, 7654 (2010). Chapter 3.

- *Quantum dynamics of dissociative chemisorption of $CH_4$ on Ni(111): Influence of the bending vibration*, G. P. Krishnamohan, R. A. Olsen, G. J. Kroes, F. Gatti, and S. Woittequand, J. Chem. Phys., in press. Chapter 4.

- *Reactive and nonreactive scattering of $N_2$ from Ru(0001): A six-dimensional adiabatic study*, C. Díaz, J. K. Vincent, G. P. Krishnamohan, R. A. Olsen, G. J. Kroes, K. Honkala, and J. K. Nørskov, J. Chem. Phys, **125**, 114706 (2006). Chapter 5.

- *Multidimensional effects on dissociation of $N_2$ on Ru(0001)*, C. Díaz, J. K. Vincent, G. P. Krishnamohan, R. A. Olsen, G. J. Kroes, K. Honkala, and J. K. Nørskov, Phys. Rev. Lett., **96**, 96102 (2006). Chapter 5.

Other publications:

- *Phase stabilities of Pd-H alloys: First-principles investigations with a statistical thermodynamics approach*, A. Marashdeh, D. E. Nanu, G. P. Krishnamohan and A. J. Böttger (article in preparation, 2010).

- *A computational study of cation-$\pi$ interaction in polycyclic systems: exploring the dependence on the curvature and electronic factors*, U. Devapriyakumar, M. Punnagai, G. P. Krishnamohan, and G. N. Sastry, Tetrahedron, **60**, 3037 (2004).

# Curriculum Vitae

I was born on 28 February of 1980 in Trivandrum, India. I passed the secondary school studies in 1995 and then chose the math group for the pre-university course with an optional subject: electronics. In 1997, I joined the University College in Trivandrum for the B.Sc. course in Chemistry. There, Dr. Sadasivan and Dr. C. Moly Merceline guided me in several theoretical/experimental sections in chemistry. My M.Sc. program was in physical chemistry which I did in the campus of Mahatma Gandhi University in Kerala, India. Dr. A. S. Padmanabhan and Dr. G. Narahari Sastry guided me in mathematical and computational chemistry respectively. After M.Sc. course I joined an engineering training center in Trivandrum to teach programming for some months.

On May 1'st of 2004, I started my Ph.D. research work in the theoretical chemistry group led by Prof. Dr. Geert-Jan Kroes in the University of Leiden. Prof. Dr. Roar A. Olsen is the other promoter. The main goal of the project is to study the role of vibrational efficacy of the different vibrational eigenstates of the methane molecule in its dissociative chemisorption on the nickel (111) surface.

In 2008 and 2009 I have assisted in the elementary quantum chemistry course for the B.Sc. students in life science and technology in the Technical University of Delft, where Dr. Martina Huber was the lecturer.

During my Ph.D. program, I have attended several winter schools and conferences. I attended the Dutch winter school in theoretical chemistry and spectroscopy in 2004, 2005 and 2006 in Belgium. In 2006, I participated in the winter school in 'computational nanoscience' held in Germany. I have been to the "Spectroscopie en Theorie" national conference in Lunteren for four times for poster presentations. In 2005, 2007 and in 2009, I have attended the GRC conferences entitled 'Dynamics at surfaces' in the USA for poster presentations.

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