Ab initio molecular dynamics calculations on reactions of molecules with metal surfaces

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Curriculum Vitae

Francesco Nattino was born on December, 26 1987 in Lecco (Italy). In 2006, he graduated from the high school Liceo Classico A. Manzoni (Lecco). He studied chemistry at the University of Milan from October 2006 to October 2011, obtaining both a bachelor and a master degree *cum laude*. In his bachelor project, he first approached the field of computational chemistry, with a molecular dynamics study of a metabotropic glutamate receptor under the supervision of Dr. Alessandro Contini and Dr. Laura Belvisi. In his master studies, he specialized in physical chemistry and joined the Chemical Dynamics Theory Group of Prof. Dr. Rocco Martinazzo and Prof. Dr. Gian Franco Tantardini. During his master project, which has been partially carried out at the Leiden Institute of Chemistry (LIC) with an Erasmus scholarship, he started working with the *ab initio* molecular dynamics (AIMD) method, investigating the dissociation of molecular hydrogen on a copper surface. In November 2011, he joined the theoretical chemistry group of the LIC as a PhD student, with Prof. Dr. Geert-Jan Kroes as his supervisor. His research project involved the use of AIMD for modeling the reaction of molecules on metal surfaces, as described in this thesis.

List of Publications

- F. Nattino, C. Díaz, B. Jackson, and G. J. Kroes, *Effect of Surface Motion on the Rotational Quadrupole Alignment Parameter of D_2 Reacting on Cu(111)*, Phys. Rev. Lett. **108**, 236104 (2012).

- F. Nattino, H. Ueta, H. Chadwick, M. E. van Reijzen, R. D. Beck, B. Jackson, M. C. van Hemert, and G. J. Kroes, *Ab Initio Molecular Dynamics Calculations versus Quantum-State-Resolved Experiments on CHD_3 + Pt(111): New Insights into a Prototypical Gas-Surface Reaction*, J. Phys. Chem. Lett. **5**, 1294 (2014).

- B. Jackson, F. Nattino, and G. J. Kroes, *Dissociative Chemisorption of Methane on Metal Surfaces: Tests of Dynamical Assumptions Using Quantum Models and Ab Initio Molecular Dynamics*, J. Chem. Phys. **141**, 054102 (2014).

- F. Nattino, A. Genova, M. Guijt, A. S. Muzas, C. Díaz, D. J. Auerbach, and G. J. Kroes, *Dissociation and Recombination of D_2 on Cu(111): Ab Initio Molecular Dynamics Calculations and Improved Analysis of Desorption Experiments*, J. Chem. Phys. **141**, 124705 (2014).

- F. Nattino, F. Costanzo, and G. J. Kroes, *N_2 Dissociation on W(110): An Ab Initio Molecular Dynamics Study on the Effect of Phonons*, J. Chem. Phys. **142**, 104702 (2015).

- F. Nattino, D. Migliorini, and G. J. Kroes, *Methane Dissociation on Pt(111): Searching for a Specific Reaction Parameter Density Functional*, In preparation.