Semi-empirical approach to the simulation of molecule-surface reaction dynamcis

Migliorini, D.

Curriculum Vitae

Davide Migliorini was born on January, 28 1990 in Crema (Italy). In 2009 he graduated at the G. Gandini high school in Lodi (Italy). From 2009 to 2014 he attended the Università degli Studi in Milano (Italy) where he obtained a bachelor degree and master degree *cum laude* in Chemistry. During his undergraduate studies he started working in theoretical chemistry and materials science focusing on the simulation of the interaction between hydrogen atoms and graphene nanoribbons under the supervision of Prof. dr. Gian Franco Tantardini and Prof. dr. Rocco Martinazzo. In 2015 he moved to Leiden (the Netherlands) to work as a PhD candidate in the group of Prof. dr. Geert-Jan Kroes at the Leiden Institute of Chemistry of Leiden University. There the focus of his work has been on the AIMD simulation of polyatomic molecules interacting with transition metal surfaces, as described in this Thesis.

List of Publications

- F. Nattino, D. Migliorini, M. Bonfanti and G. J. Kroes, "Methane Dissociation on Pt(111): Searching for a Specific Reaction Parameter Density Functional", *J. Chem. Phys.*, 144, 044702 (2016).

- D. Migliorini, F. Nattino and G. J. Kroes,"Application of van der Waals Functionals to the Calculation of Dissociative Adsorption of N_2 on W(110) for Static and Dynamic Systems", *J. Chem. Phys.*, 144, 084702 (2016).

- F. Nattino, D. Migliorini, G. J. Kroes, E. Dombrowski, E. A. High, D. R. Killelea and A. L. Utz, "Chemically Accurate Simulation of a Polyatomic Molecule-Metal Surface Reaction", *J. Chem. Phys. Lett.*, 7, 2402 (2016).

- D. Migliorini, H. Chadwick, F. Nattino, A. Gutiérrez-González, E. Dombrowski, E. A. High, H. Guo, A. L. Utz, B. Jackson, R. D. Beck, and G. J. Kroes, "Surface Reaction Barriometry: Methane Dissociation on Flat and Stepped Transition-Metal Surfaces", *J. Chem. Phys. Lett.*, 8, 4177 (2017).

- H. Chadwick, D. Migliorini and G. J. Kroes, "CHD_3 Dissociation on Pt(111): A Comparison of the Reaction Dynamics Based on the PBE Functional and on a Specific Reaction Parameter Functional", *J. Chem. Phys.*, 149, 044701 (2018).

- H. Chadwick, A. Gutiérrez-González, D. Migliorini, R. D. Beck and G. J. Kroes, "Incident Angle Dependence of CHD_3 Dissociation on the Stepped Pt(211) Surface", *J. Phys. Chem. C*, 122, 19652 (2018).

- D. Migliorini, H. Chadwick and G. J. Kroes, "Methane on a Stepped Surface: Dynamical Insights on the Dissociation of CHD_3 on Pt(111) and Pt(211)", *J. Chem. Phys.*, 149, 094701 (2018).

- N. Gerrits, D. Migliorini and G. J. Kroes, "Dissociation of CHD_3 on Cu(111), Cu(211) and single atom alloys of Cu(111)", *J. Chem. Phys*, 149, 224701 (2018).

- D. Migliorini, F. Nattino, A. K. Tiwari and G. J. Kroes, "HOD on Ni(111): Ab Initio Molecular Dynamics Prediction of Molecular Beam Experiments", *J. Chem. Phys*, 149, 244706 (2018).