Hydrogen dissociation on metal surfaces: A semi-empirical approach

Nour Ghassemi, E.

Curriculum Vitae

Elham Nour Ghassemi was born on March, 21 1980 in Tabriz (Iran). In 1999, she was graduated in Mathematics and Physics from Tohid high school, Tabriz, Iran. She received her BSc degree in Solid State Physics from Azerbijan University, Tabriz, Iran. After receiving her bachelor's degree in 2003, she studied Solid State Physics and Electronics at the University of Tabriz from 2003 to 2005, obtaining her master degree. She started working at the lab located in Isfahan University of Technology, as a teacher and research assistance for three years. On September 2008, she moved to Stockholm, Sweden, where she got admitted to work as a research assistance at Stockholm University under supervision of Prof. dr. Åsa Larson and Dr. Jonas Larson in the faculty of science in theoretical physics and the molecular physics department. She received a second master degree in 2011 and continued her collaboration with Stockholm University until 2012. On January 2014, she joined the group of Prof. dr. Geert-Jan Kroes at the Leiden Institute of Chemistry of Leiden University, The Netherlands as a PhD candidate. Her research was funded by an ERC Advanced grant. Her research led to a number of publications and this thesis.

List of Publications

1. J. Larson, E. Nour Ghassemi and Å. Larson "Anomalous Molecular Dynamics in the Vicinity of a Conical Intersection" *EPL (Europhysics Letters)* 101, 43001 (2013).

2. E. Nour Ghassemi, J. Larson, Å. Larson, "A Diabatic Representation of the Two Lowest Electronic States of Li_3" *The Journal of Chemical Physics* 140, 154304 (2014).

3. E. Nour Ghassemi, M. Wijzenbroek, M. F. Somers, and G. J. Kroes, "Chemically Accurate Simulation of Dissociative Chemisorption of D_2 on Pt(111)" *Chemical Physics Letters*, 683, 329-335 (2017).

4. E. Nour Ghassemi, M. F. Somers and G. J. Kroes, "Test of the Transferability of the Specific Reaction Parameter Functional for H_2 + Cu(111) to D_2 + Ag(111)" *The Journal of Physical Chemistry C*, 122, 22939-22952 (2018).

5. E. Nour Ghassemi, E. W. F. Smeets, M. F. Somers, G. J. Kroes, I. M. N. Groot, L. B. F. Juurlink, G. Füchsel, "Transferability of the Specific Reaction Parameter Density Functional for H_2 + Pt(111) to H_2 + Pt(211)" *The Journal of Physical Chemistry C* 123(5), 2973-2986 (2019).

6. E. Nour Ghassemi, M. F. Somers, and G. J. Kroes, "Assessment of Two Problems of Specific Reaction Parameter Density Functional Theory: Sticking and Diffraction of H_2 on Pt(111)" *The Journal of Physical Chemistry C* 123(16), 10406-10418 (2019).

Afterword

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