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Beyond the Born-Oppenheimer static surface model for molecule-surface reactions

Spiering, P.

Citation

Spiering, P. (2019, December 16). *Beyond the Born-Oppenheimer static surface model for molecule-surface reactions*. Retrieved from <https://hdl.handle.net/1887/81817>

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Author: Spiering, P.

Title: Beyond the Born-Oppenheimer static surface model for molecule-surface reactions

Issue Date: 2019-12-16

Beyond the
Born-Oppenheimer Static Surface Model
for Molecule-Surface Reactions

PROEFSCHRIFT

ter verkrijging van
de graad van Doctor aan de Universiteit Leiden,
op gezag van Rector Magnificus prof. mr. C. J. J. M. Stolker,
volgens besluit van het College voor Promoties
te verdedigen op maandag 16 december 2019
klokke 13:45 uur

door

Paul Spiering
geboren te Bergschenhoek, Nederland, 1990

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ISBN: 978 90 361 0597 2

The research described in this thesis has been performed at the Theoretical Chemistry group of the Leiden Institute of Chemistry (Einsteinweg 55, 2333 CC, Leiden). This work has been supported by the Netherlands Organisation for Scientific Research (NWO) via Vidi grant no. 723.014.009.

Typeset with L^AT_EX.

Figures and cover made with L^AT_EX, gnuplot and GLE.

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Acronyms

AIMD *ab-initio* molecular dynamics.

BOA Born-Oppenheimer approximation.

COM center of mass.

CRP corrugation reducing procedure.

DFPT density functional perturbation theory.

DFT density functional theory.

DOF degrees of freedom.

ehp electron-hole pair.

GGA generalised gradient approximation.

GLE generalized Langevin equation.

HEG homogeneous electron gas.

KS Kohn-Sham.

LDA local density approximation.

LDFA local density friction approximation.

Acronyms

MD molecular dynamics.

MDEF molecular dynamics with electronic friction.

MEP minimum energy path.

NN neural network.

ODF orbital-dependent friction.

PES potential energy surface.

QC quasi-classical.

RMSE root-mean-square error.

SCM static corrugation model.

SRP specific reaction parameter.