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

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Contents

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.

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.