

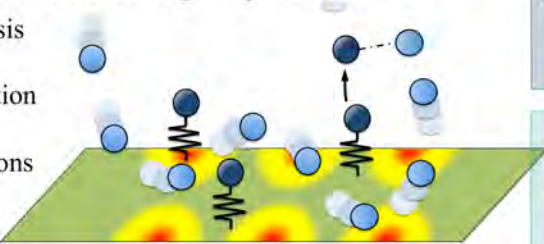


Phonon and electron excitations in diatom abstraction from metal surfaces

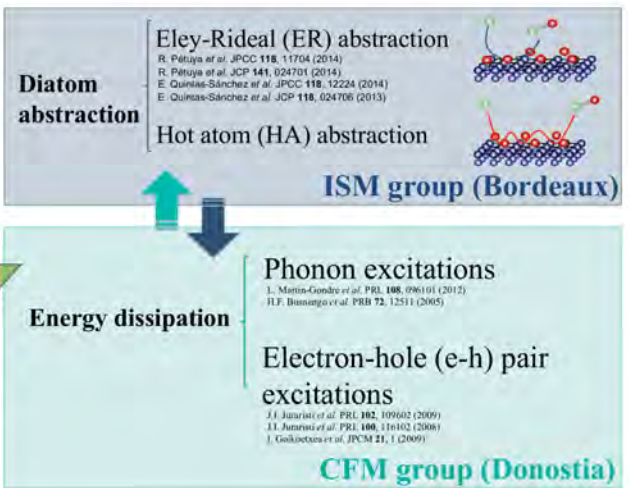
PROBLEM

Gas-surface elementary reactions play a prominent role in a huge variety of natural and technological processes:

- heterogeneous catalysis
- nano-structuration
- surface functionalization
- hydrogen storage
- plasma-wall interactions in nuclear fusion
- atmospheric entries...



Aim of the project: Rationalization of N₂ and H₂ recombination processes on W(100) and W(110) surfaces



METHODOLOGY

Classical molecular dynamics simulations *within* Adiabatic DFT-based multidimensional PES

Detailed view of the chemical reaction

$$\frac{d^2 \mathbf{r}_i}{dt^2} = -\frac{1}{m_i} \nabla_i V$$

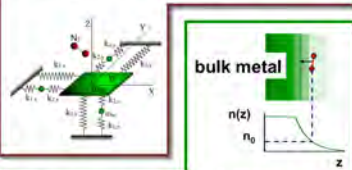
N atoms + surface :
 Multi-adsorbate PES

$$V(\{\mathbf{r}_i\}) = \sum_{i=1}^N V^{3D}(\mathbf{r}_i) + \sum_{i=1}^N \sum_{j>1}^N V^{6D}(\mathbf{r}_i, \mathbf{r}_j)$$

D.V. Shalashilin et al. JCP 110, 11038 (1999)

Implementation of nonadiabaticity

Phonon excitations: GLO model
 Generalized Langevin Oscillator
 S. A. Adelman, JCP 71, 4471 (1979)
 J. Tully, JCP 73, 1975 (1980)
 H. F. Busnengo et al. PRB 72, 125411 (2005)

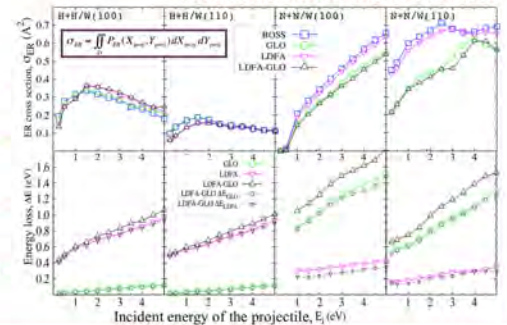


e-h pair excitations: LDFA model
 Local Density Friction Approximation
 J.J. Juarez et al. PRL 100, 116102 (2008)

EXPECTED RESULTS

- Analysis of ER and HA reaction channels
- Prediction of the influence on reactivity
 - phonons excitations
 - e-h pair excitations
- Prediction of the influence on energy exchange
 - phonons excitations
 - e-h pair excitations

First results: Phonon and electron excitations in ER abstraction from metal surfaces



CONCLUSION

IN GENERAL

Advance in the comprehension of microscopical processes on gas-surface reactions

IN PARTICULAR

W = main candidate for the divertors on the ITER fusion reactors

prediction of the degradation of internal walls of fusion reactor crucial to allow sufficiently long lifetimes for the industrial applications

H+H/W and N+N/W = model systems for plasma-wall interactions (ITER, atmospheric entry)

prediction of the energy transfers major issue for interstellar reactions and for the control of plasma/wall interactions

