

## Séminaire de Chimie Théorique

Salle de réunion groupe THEO, bat. A12

Lundi 20 Avril à 11 :00

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## Scattering of atoms and molecules from periodic surfaces: Exploring new frontiers

New experimental and theoretical developments are giving a new impulse to the study of atomic and molecular scattering phenomena. In this talk, we will discuss few examples of these scattering phenomena. First, we will discuss the scattering of noble gases from metal surfaces. We will show that, nowadays, new van der Waals functionals [1,2] allow one to perform accurate simulations using density functional theory (DFT) based potential energy surfaces (PES). Second, we will show results on atomic and molecular scattering under fast grazing incidence (FGI) conditions. Measured experimentally for the first time in 2007 [3,4], FGI has revealed as a very promising tool to study molecule/surface interactions [5,6]. We will discuss recent theoretical results on this topic.

[1] M. Dion et al Phys. Rev. Lett. 92, 246401 (2004)

[2] J. Klimes et al Phys. Rev. B 83, 195131 (2011)

[3] A. Schüller et al Phys. Rev. Lett. 98, 016103 (2007)

[4] P. Rousseau et al Phys. Rev. Lett. 98, 016104 (2007)

[5] C. Díaz et al Phys. Rev. Lett. 103, 013201 (2009)

[6] H. Winter et al Prog. Surf. Sci. 86, 169 (2011)

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