

MAR14-2013-020123

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

Dynamics of irradiation: from molecules to nano-objects and from material science to biology¹

ERIC SURAUD, Laboratoire Physique Theorique, Universite Paul Sabatier Toulouse 3

We discuss microscopic mechanisms of irradiation in clusters and molecules. We consider the case of isolated molecules/clusters [1] possibly in contact with an environment [2]. We use Time Dependent Density Functional Theory (for electrons) coupled to Molecular Dynamics (for ions) and follow explicitly in time both irradiation and response of the system. Examples are taken from free metal clusters, from fullerenes, from molecules of biological interest and from clusters deposited on a surface or embedded in a matrix [3,4]. We analyse in particular the properties of emitted electrons (photo electron spectra, angular distributions...), which constitute a key tool of analysis of the properties of irradiated clusters and molecules [5]. We also discuss the possibility of pump and probe scenarios (opening the road to manipulation at the molecular scale) with help of dedicated laser pulses, exploring high laser frequencies towards the FEL regime and very short times scales down towards the attosecond domain.

[1] F. Calvayrac et al, Phys. Reports (2000)4932

[2] P. M. Dinh et al, Phys. Reports (2009) 433

[3] Z.P. Wang et al, Int. J. Mass Spect. (2009) 14304

[4] U. F. NdongmuoTaffoti et al, Eur. Phys. J. D (2010) 1315

[4] Th. Fennel et al, Rev. Mod. Phys. (2010) 1793.

¹Work supported by Institut Universitaire de France, Agence nationale de la Recherche and European ITN network CORINF.