

Abstract Submitted
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Dynamics of irradiation: from molecules to nano-objects and from material science to biology ERIC SURAUD, PHUONG MAI DINH, Laboratoire de Physique Théorique, Université Paul Sabatier 118 Route de Narbonne, 31062 Toulouse cedex, France, PAUL-GERHARD REINHARD, Institut fuer Theoretisch Physik, Universitaet Erlangen Staudstrasse 7, D91058 Erlangen, Germany — We discuss microscopic mechanisms of irradiation in clusters and molecules considering the case of isolated molecules/clusters [1] and/or in an environment [2]. We use Time Dependent Density Functional Theory (for electrons) coupled to Molecular Dynamics (for ions) and follow explicitly in time irradiation and response of the system. Examples are taken from free metal clusters, fullerenes, molecules of biological interest and clusters deposited on a surface or embedded in a matrix [3,4]. We analyse in particular properties of emitted electrons (photo electron spectra, angular distributions...) which provide a key tool of analysis of properties of irradiated clusters and molecules [5]. We also discuss pump and probe scenarios (opening the road to manipulation at the molecular scale) with help of dedicated laser pulses, exploring in particular very short times scales down towards the attosecond domain.

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