

APS March Meeting 2020

View Abstract

CONTROL ID: 3309447

TITLE: Ab-initio photo-ionization dynamics without continuum states

Abstract Body: Photo-ionization underpins a range of spectroscopies central to the study of structural and dynamical properties of matter in the gas and solid phases. In solid state physics angular resolved photoelectron spectroscopy (ARPES) and time-resolved (tr) ARPES are the most prominent techniques. Leveraging the flexibility offered by real-space methods we developed a technique, based on the real-time formulation of time-dependent density functional theory (TDDFT), to simulate ARPES and tr-ARPES ab-initio without explicit reference to continuum states [1]. I will present the theory, the algorithm involved in the implementation and some of the most representative applications and predictions.

[1] U. De Giovannini, H Hübener, A. Rubio, JCTC. 13, 265 (2017).

PRESENTATION TYPE: Oral

UNIT: 16.0 GENERAL THEORY, COMPUTATIONAL PHYSICS (DCOMP)

SORTING CATEGORY: 16.01.09 Real-space methods for the electronic structure problem: new algorithms and applications (DCOMP)

Category Type: Computational

AUTHORS (FIRST NAME, LAST NAME): Umberto De Giovannini¹

INSTITUTIONS (ALL): 1. Max Planck Inst Structure & Dynamics of Matter

Teams: (none)

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