Prof. Mauro Stener
Full professor of Physical Chemistry

Personal information

Born in Trieste, June, 13th 1967
Italian citizen, married, one daughter and one son.
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Mauro Stener, graduated in chemistry in 1992 at Trieste University with score 110/110 cum laude. In 1995 he got the PhD in Theoretical Chemistry. In 1996 he spent one year as postdoc at Technischen Universität München, at the Lehstuhl fur Theoretische Chemie. From 1998 assistant professor, from 2006 associate professor and from 2019 full professor of physical chemistry at Trieste University.

Research

The research activity of Prof. Mauro Stener is in the field of theoretical chemistry, and essentially takes place along three themes: 1) Development of new methods for DFT and TDDFT 2) Theoretical study of metal clusters 3) Theoretical study of molecular photoionization processes. The results obtained from the research activity have been collected up to now in 211 publications and in 113 communications to conferences. 5102 citations, h-index = 39 (source: WOS)

- Development of new methods for DFT and TDDFT

In our group we have a long collaboration with SCM (Amsterdam) since we are developers of the ADF (now AMS) suite of programs. In particular in ADF we have implemented core electron excitations [1], the polTDDFT method to calculate the optical properties of very large systems [2], and the Hybrid Diagonal Approximation (HDA) [3] to speedup TDDFT calculations with hybrid kernels and Slater Type Orbitals (STO) basis sets. We also worked on analysis tools for TDDFT, as the fragment analysis [4] and the ICM-OS [5]

- Theoretical study of metal clusters.

We are in particular interested in the optical properties of metal clusters, such as plasmonic behaviors [6], circular dichroism [7], rebirth of plasmons thanks to ligand effects [8] and alloying effects [9]. Most of such studies are in collaboration with CNR in Pisa (A. Fortunelli).

- Theoretical study of molecular photoionization processes.

We have participated to the development of the Tiresia code, for the treatment of molecular photoionization with explicit treatment of the electronic continuum spectrum. The non-bound boundary conditions are obeyed since non-conventional B-spline basis functions are employed. In particular we developed and currently employ the TDDFT B-spline part of the code [10].

10 selected publication

[1] M. Stener, G. Fronzoni and M. de Simone " Time Dependent Density Functional Theory of Core Electrons Excitations " Chem. Phys. Lett., 373 (2003) 115.

[2] Oscar Baseggio, Giovanna Fronzoni and Mauro Stener "A New Time Dependent Density Functional Algorithm for Large Systems and Plasmons in Metal Clusters" J. Chem. Phys., 143 (2015) 024106.

[3] Marco Medves, Luca Sementa, Daniele Toffoli, Giovanna Fronzoni, Alessandro Fortunelli, and Mauro Stener "An Efficient Hybrid Scheme for Time Dependent Density Functional Theory" J. Chem. Phys., 152 (2020) 184102 (1-10).

[4] Luca Sementa, Giovanni Barcaro, Oscar Baseggio, Martina De Vetta, Amala Dass, Edoardo Aprà, Mauro Stener, Alessandro Fortunelli "Ligand-Enhanced Optical Response of Gold Nanomolecules and its Fragment Projection Analysis: the Case of $Au_{30}(SR)_{18}$", J. Phys. Chem. C 121 (2017) 10832 – 10842.

[5] Theivendran, Shevanuja; Chang, Le; Mukherjee, Aneek; Sementa, Luca: Stener, Mauro; Fortunelli, Alessandro; Dass, Amala "Principles of Optical Spectroscopy of Aromatic Alloy Nanomolecules: $Au_{36-x}Ag_x(SPh\text{-}tBu)_{24}$" J. Phys. Chem. C 122, (2018) 4524-4531.

[6] GiovanniMaria Piccini, Remco W. A. Havenith, Ria Broer and Mauro Stener, "Gold nanowires: a Time Dependent Density Functional assessment of plasmonic behaviour" J. Phys. Chem. C, 117 (2013) 17196 – 17204.

[7] Daniele Toffoli, Andrea Russi, Giovanna Fronzoni, Emanuele Coccia, Mauro Stener, Luca Sementa and Alessandro Fortunelli "Circularly Polarized Plasmons in Chiral Gold Nanowires via Quantum Mechanical Design" J. Phys. Chem. Lett. 2021, 12, 5829−5835

[8] L. Sementa, G. Barcaro, A. Dass, M. Stener, and A. Fortunelli "Designing Ligand-Enhanced Optical Adsorption of Thiolated Gold NanoClusters" Chem. Comm. 51 (2015) 7935 – 7938

[9] Nicola Danielis, Lorena Vega, Giovanna Fronzoni, Mauro Stener, Albert Bruix and Konstantin Neyman "AgPd, AuPd and AuPt nanoalloys with Ag- or Au-rich compositions: Modeling the interplay between chemical ordering and optical properties" J. Phys. Chem. C 2021, 125, 31, 17372–17384

[10] M. Stener, G. Fronzoni and P. Decleva "Time Dependent Density Functional Theory for molecular photoionization with non-iterative algorithm and multicenter B-spline basis set: CS_2 and C_6H_6 case studies" J. Chem. Phys., 122 (2005) 234301.

Managing experience

- Vice Director of the Department of Chemical Sciences of UniTS from November 2008 to November 2010 and of the Department of Chemical and Pharmaceutical Sciences of UniTS from September 2015 to July 2018.
- University representative in the Board of Directors of the INSTM consortium from November 2009 to November 2015.
- Coordinator of the PhD in Chemistry from June 2012 to October 2017.
- From September 1st 2018 to August 31st 2021 Director of the Department of Chemical and Pharmaceutical Sciences of the University of Trieste.
- From 1st November 2018 to October 31st 2021, member of the Academic Senate of the University of Trieste.

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