New TDDFT Algorithms and Analysis Tools for Optical Properties of Large Systems

MAURO STENER[1], Daniele Toffoli[1], Pierpaolo D'Antoni[1], Marta Monti[2], Marco Medves[1], Luca Sementa[3] and Alessandro Fortunelli[3]

[1]*Dipartimento di Scienze Chimiche e Farmaceutiche, Università di Trieste, Via Giorgieri 1, Trieste (Italy)*
[2]*International Center for Theoretical Physics, Strada Costiera 11, Trieste (Italy)*
[3]*CNR, ICCOM & IPCF, Via Moruzzi 1, Pisa (Italy).*
stener@units.it

ABSTRACT

A recent algorithm to solve the TDDFT equations in the space of the density fitting auxiliary basis set has been developed and implemented in ADF/AMS [1]. The TDDFT equations are recast to a non-homogeneous linear system, whose size is much smaller than in Casida formulation, allowing to calculate a wide portion of the absorption spectrum for large systems. The method extracts the spectrum from the imaginary part of the polarizability at any given photon energy, avoiding the bottleneck of Davidson diagonalization. The new algorithm also benefits from a recent very efficient extension to hybrid functionals and is supported by many analysis tools. Recent applications to ligand protected and chiral metal clusters will show the potentiality of the method.

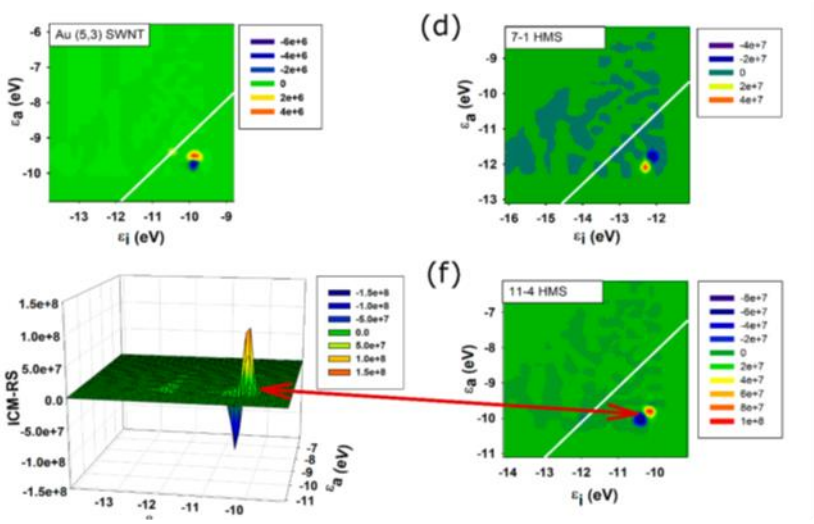

Figure 1: ICM-RS analysis tools for CD.

References

[1] O. Baseggio, G. Fronzoni and M. Stener *J. Chem. Phys.*, **2015**, *143*, 024106.