



**UNIVERSITÀ
DEGLI STUDI
DI TRIESTE**

Fast and accurate excitation and CD spectra of large systems with PolTDDFT: from molecular to plasmonic regimes

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PolTDDFT: why yet another TDDFT scheme?

Theory: for large metal nanoclusters (up to 1000 atoms) TDDFT is the only possibility!

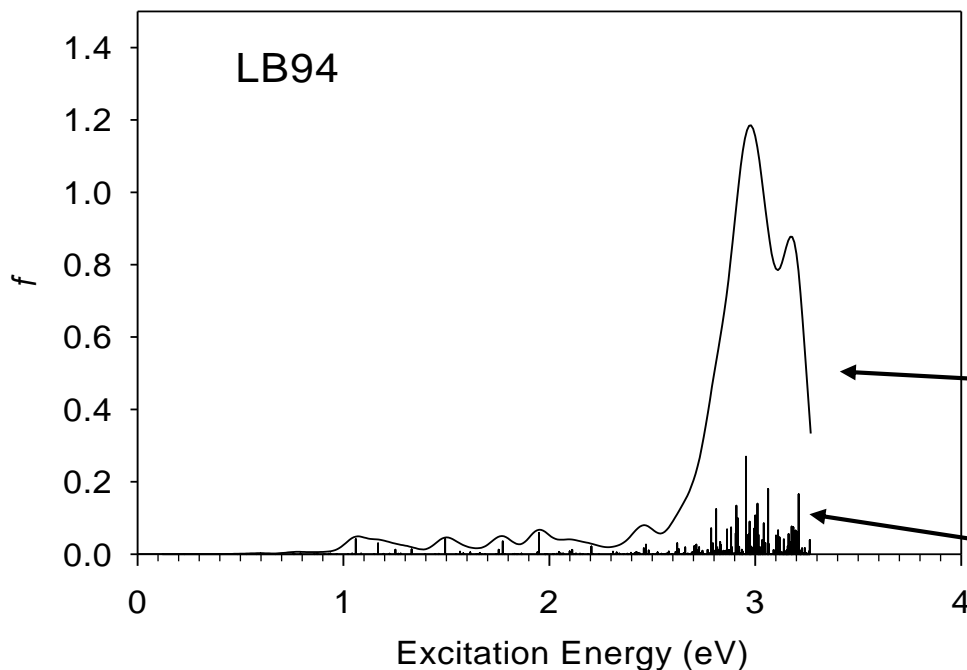
- 1. Efficiency:** the **polTDDFT** is an alternative to **Casida** scheme, avoid **Davidson diagonalization!** Very competitive when too many excited states are needed.
- 2. Accuracy/Efficiency:** **Hybrid** functionals (B3LYP), new Hybrid Diagonal Approximation (**HDA**)
- 3. Accuracy/Efficiency:** optimization of density **fitting basis** set.
- 4. Validation:** comparison with experiment. Monolayer-Protected Cluster (**MPC**) structure and optical properties well characterized.
- 5. Selected Applications:** dichroism in nanoplasmonics
- 6. Input example/explanation**

TDDFT Equations: Casida approach

$$\Omega \mathbf{F}_I = E_I^2 \mathbf{F}_I$$

Casida formulation: Diagonalization of Ω matrix furnishes discrete excitation energies and intensities $\text{dim} = N_{\text{occ}} * N_{\text{virt}}$

$[\text{Au}_{172}]^{4+}$ Cubic TDDFT
optimized geometry at LDA level



STO TZP, closed shell:

$N_{\text{occ}}=1632$ $N_{\text{virt}}=3872$

$\text{dim}(\Omega)=6.3 \cdot 10^6$

Gaussian broadening

TDDFT results, lowest
 n eigenvalues

Linear response : general theory

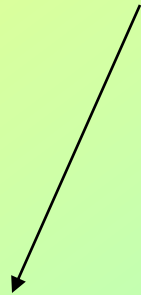
$$V_{EXT}(\vec{r}, \omega)$$

External TD perturbation, with ω
frequency (dipole)

$$\rho^{(1)}(\vec{r}, \omega)$$

Induced density by the external field

$$\rho^{(1)}(\vec{r}, \omega) = \int d\vec{r}' \chi(\vec{r}, \vec{r}', \omega) V_{EXT}(\vec{r}', \omega)$$



Dielectric susceptibility, not easy to calculate

TDDFT: general theory

TDDFT: instead of χ , use χ_{KS} of a model system of non-interacting electrons and a modified external potential: V_{SCF}

$$\rho^{(1)}(\vec{r}, \omega) = \int d\vec{r}' \chi_{\text{KS}}(\vec{r}, \vec{r}', \omega) V_{\text{SCF}}(\vec{r}', \omega)$$

Coupled, but linear!

$$V_{\text{SCF}}(\vec{r}, \omega) = V_{\text{EXT}}(\vec{r}, \omega) + \underbrace{\int d\vec{r}' \frac{\rho^{(1)}(\vec{r}', \omega)}{|\vec{r} - \vec{r}'|} + \frac{dV_{\text{XC}}^{\text{LDA}}(\rho(\vec{r}))}{d\rho(\vec{r})} \rho^{(1)}(\vec{r}, \omega)}_{K(r, r') \text{ (kernel)}}$$

$K(r, r')$ (kernel)

Efficiency: polTDDFT direct (not iterative) algorithm

Exploit linearity of the problem:

$$\delta V = K \rho^{(1)} \longrightarrow \text{defines the kernel } K$$

$$\rho^{(1)} = \chi_{KS} V_{SCF} \longrightarrow \text{defines the susceptibility } \chi_{KS}$$

$$V_{SCF} = V_{EXT} + \delta V$$

The Response Equation becomes:

$$\boxed{\boxed{[1 - \chi_{KS} K] \rho^{(1)} = \chi_{KS} V_{EXT}}}$$

$$\rho^{(1)} = \sum_{\mu}^{fit} b_{\mu} f_{\mu}$$

To solve : represent the response equation in the **auxiliary density fitting basis functions**, dimension of fitting set (**density-based** formulation). At variance with **density-matrix** Casida formulation. For $[\text{Au}_{172}]^{4+}$ $\dim(1 - \chi_{KS} K) = 5848$ (instead of $6.3 \cdot 10^6$)!!!

O. Baseggio, G. Fronzoni and M. Stener, J. Chem. Phys., 143 (2015) 024106

O. Baseggio, M. De Vetta, G. Fronzoni, M. Stener and A. Fortunelli, Int. J. Quantum Chem., 116 (2016) 1603

Extract the spectrum from polarizability:

$$\alpha_{pq}(\omega) = \int \rho_p^{(1)}(\omega, \bar{r}) q d\bar{r}$$

$$\alpha(\omega) = \frac{1}{3} \sum_{q=1}^3 \alpha_{qq}(\omega)$$

$$\sigma(\omega) = \frac{4\pi\omega}{c} \Im[\alpha(\omega)]$$

The first order density $\rho^{(1)}$ calculated from TDDFT equations, for each photon energy ω with $\omega = \omega_R + i\omega_I$ the imaginary part corresponds to lorentzian HWHM broadening.
basis set: auxiliary density fitting functions optimized for POLTTDFT must be employed!

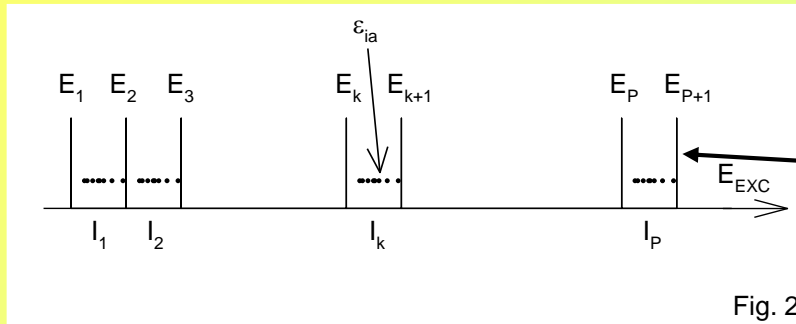
$$\rho^{(1)} = \sum_{\mu}^{fit} b_{\mu} f_{\mu}$$

$$[1 - \chi_{KS} K] \rho^{(1)} = \chi_{KS} V_{EXT} \quad [\mathbf{S} - \mathbf{M}(\omega)] \mathbf{b} = \mathbf{d}(\omega)$$

The “only” problem is to calculate efficiently χ_{KS} !

Change the double sum:

$$\chi_{KS}(\omega, \bar{r}, \bar{r}') = \sum_i^{Nocc} \sum_a^{Nvirt} \varphi_i(\bar{r}) \varphi_a(\bar{r}) \frac{4\varepsilon_{ia}}{\omega^2 - \varepsilon_{ia}^2} \varphi_a(\bar{r}') \varphi_i(\bar{r}') = \sum_i^{Nocc} \sum_a^{Nvirt} \Theta_{ia}(\bar{r}) \lambda_{ia}(\omega) \Theta_{ia}(\bar{r}')$$



Cut-off crucial input choice for polTDDFT: include relevant excitations but avoid unnecessary ones to prevent numerical errors propagation.

The energy grid consists of $P+1$ knots: $\{E_k\}_{k=1,\dots,P+1}$
and are defined P intervals: $I_k = [E_k, E_{k+1}), k = 1, \dots, P$

Now it is possible to change the double sum of previous equation (13) as follows:

$$\chi_{KS}(\omega, \bar{r}, \bar{r}') = \sum_{k=1}^P \sum_{\varepsilon_{ia} \in I_k} \Theta_{ia}(\bar{r}) \lambda_{ia}(\omega) \Theta_{ia}(\bar{r}')$$

$$\chi_{KS}(\omega, \bar{r}, \bar{r}') = \sum_{k=1}^P \frac{4\bar{E}_k}{\omega^2 - \bar{E}_k^2} \sum_{\varepsilon_{ia} \in I_k} \Theta_{ia}(\bar{r}) \Theta_{ia}(\bar{r}')$$

Build the matrix:

TDDFT equation: $[\mathbf{S} - \mathbf{M}(\omega)]\mathbf{b} = \mathbf{d}(\omega)$

$$M(\omega)_{\mu\nu} = \sum_{k=1}^P s_k(\omega) \sum_{\varepsilon_{ia} \in I_k} \langle f_\mu | \Theta_{ia}(\bar{r}) \rangle \langle \Theta_{ia}(\bar{r}') | K | f_\nu \rangle = \sum_{k=1}^P s_k(\omega) G_{\mu\nu}^k$$

$$s_k(\omega) = \frac{4\bar{E}_k}{\omega^2 - \bar{E}_k^2}$$

With this scheme, the \mathbf{M} matrix is calculated at each photon energy ω , simply as a linear combination of matrices \mathbf{G}^k with coefficients $s_k(\omega)$.

The calculation of χ_{KS} is fast (just sum of matrices) and small (over the fitting functions)!

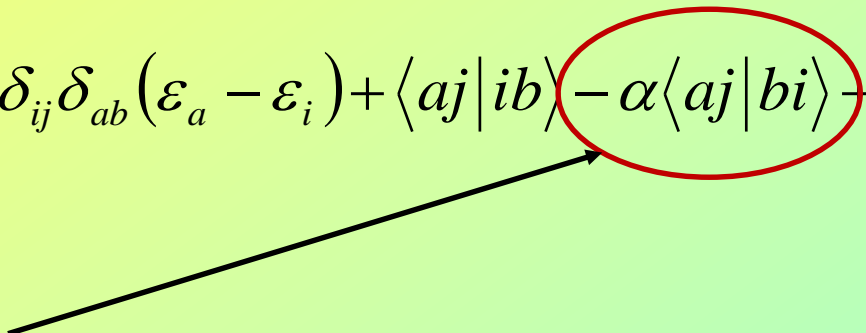
Approximations: imaginary broadening and energy discretization.

Accuracy/Efficiency: Hybrid Diagonal Approximation (HDA)

To introduce HDA is convenient to start from RPA equations:

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix}$$

For hybrid kernels the matrix elements takes this form, α fraction of non-local exchange

$$A_{ia,jb} = \delta_{ij} \delta_{ab} (\varepsilon_a - \varepsilon_i) + \langle aj | ib \rangle - \alpha \langle aj | bi \rangle - (1 - \alpha) \langle a | \frac{\partial V_{xc}}{\partial \rho} j^* b | i \rangle$$


Kernel non-local exchange elements: very demanding when non-gaussian basis are employed!

Hybrid Diagonal Approximation (HDA)

HDA consists to consider only the **diagonal** exchange elements:

$$A_{ia,jb} = \delta_{ij} \delta_{ab} (\varepsilon_a - \varepsilon_i - \Delta_{ia}) + \langle aj | ib \rangle + \langle a | \frac{\partial V_{xc}}{\partial \rho} j^* b | i \rangle$$

$$\Delta_{ia} = \alpha \langle ai | ai \rangle + \alpha \langle a | \frac{\partial V_{xc}}{\partial \rho} i^* a | i \rangle$$

The **diagonal** exchange elements are few and cheap to calculate, even for non-gaussian basis set. At present calculated numerically. Next release AMS2023: also calculated analytically with fitting (Resolution of the Identity) (Pierpaolo D'Antoni TCCM master thesis, paper in preparation). Speedup factor of 30 by RI!!!

HDA is a general approximation, it has been implemented (AMS2021) for both Casida and polTDDFT algorithms!

Hybrid Diagonal Approximation (HDA)

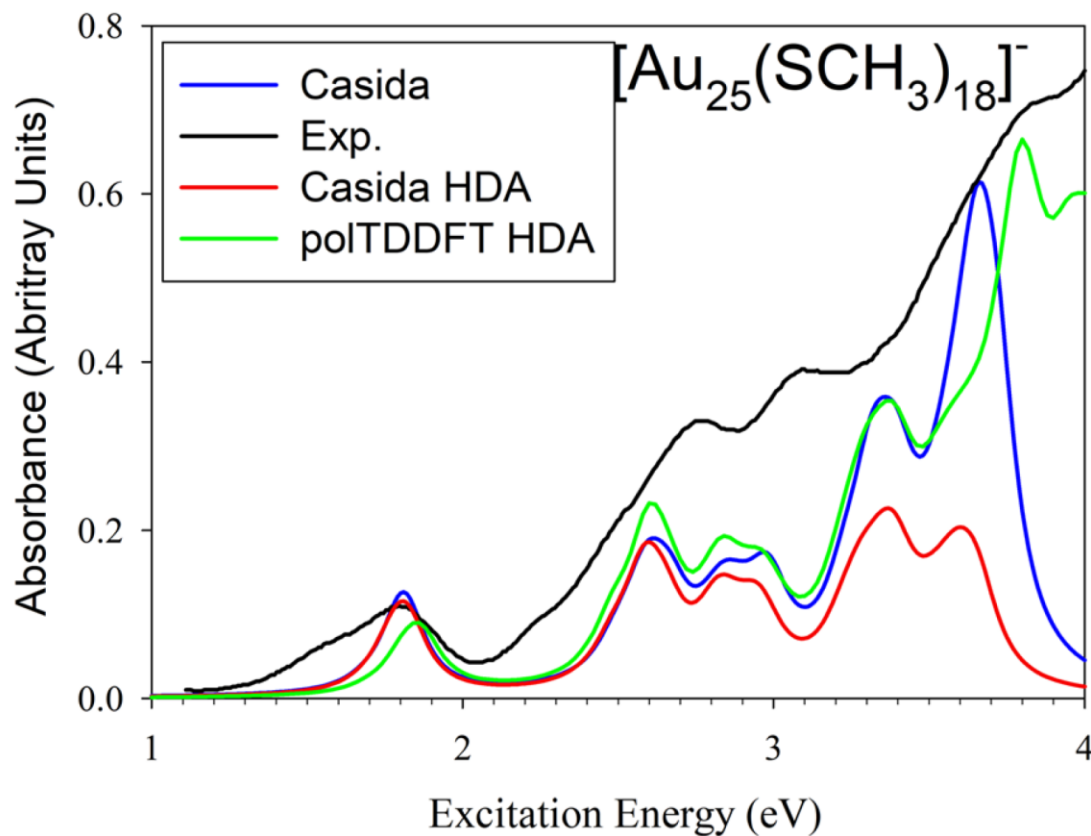


FIG. 3. Valence excitation spectra of $[\text{Au}_{25}(\text{SCH}_3)_{18}]^-$. Calculated profile with the Casida approach (blue line), Casida HDA (red line), and polTDDFT (green line), broadened with HWHM = 0.075 eV and experimental data³⁷ (black line).

Timing (24 cores)

Casida: 61 h up 3.7 eV

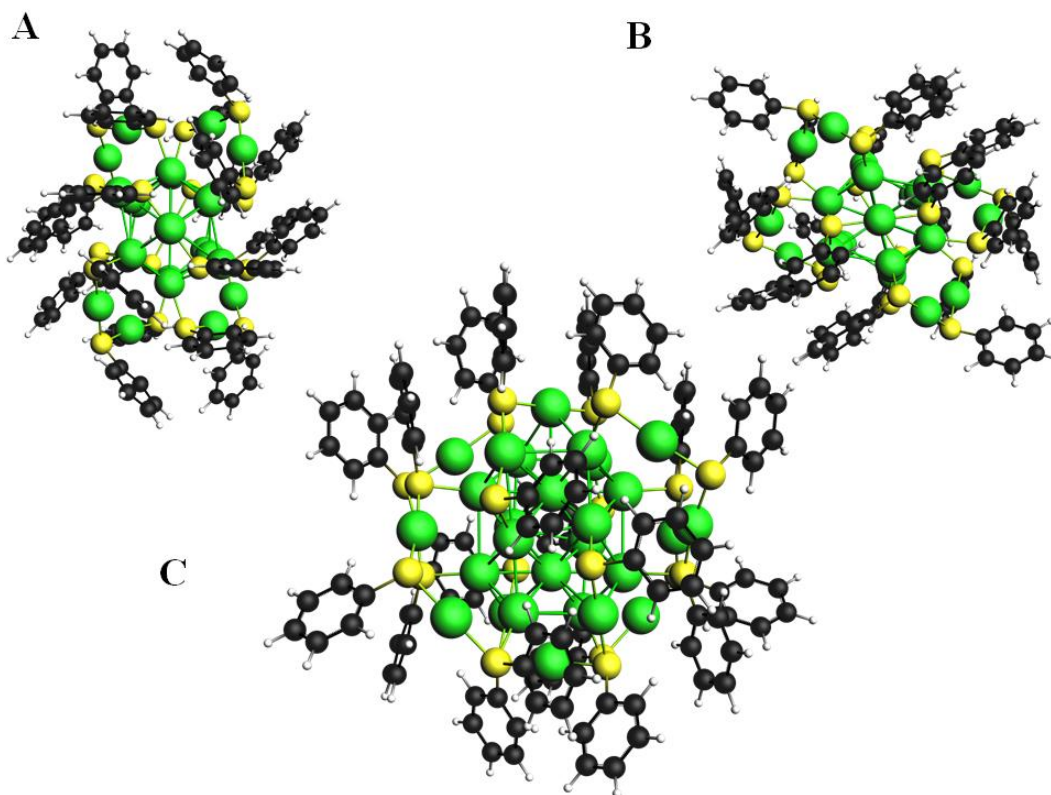
Casida HDA: 9 h up
3.7 eV

polTDDFT: 16 h up to
5eV

Hardware: HP ProLiant DL580 Gen10 server Intel®Xeon®Gold 6140 CPU @ 2.30 GHz, 728 GB of RAM

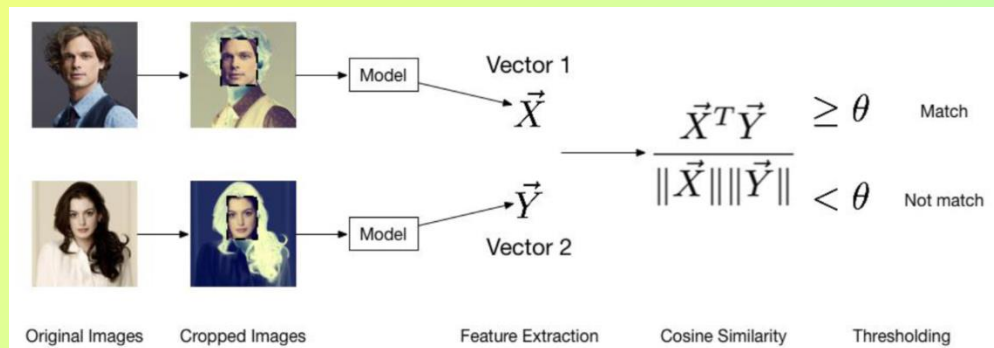
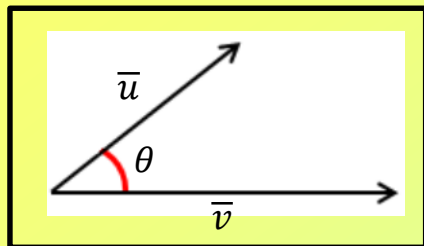
Hybrid Diagonal Approximation (HDA)

	$[\text{Au}_{25}(\text{SCH}_3)_{18}]^-$	$\text{Au}_{28}(\text{SC}_6\text{H}_5)_{20}$
Atoms	115	268
polTDDTFT HDA numerical	16h	84h
polTDDTFT HDA fitted		3h



Efficiency/Accuracy: POLTDDFT fitting basis set

$$\vec{v} \cdot \vec{u} = |\vec{v}| |\vec{u}| \cos(\theta) \Rightarrow \cos(\theta) = \frac{\vec{v} \cdot \vec{u}}{|\vec{v}| |\vec{u}|}$$



- 73 elements of the periodic table approx. 2 millions spectra analyzed
- High spread of the pol-TDDFT method in particular for “large” systems
- High accuracy and robustness included in AMS-2021

1 H Hydrogen 1.008																	2 He Helium 4.003				
3 Li Lithium 6.941	4 Be Beryllium 9.012															5 B Boron 10.811	6 C Carbon 12.011	7 N Nitrogen 14.007	8 O Oxygen 15.999	9 F Fluorine 18.998	10 Ne Neon 20.180
11 Na Sodium 22.990	12 Mg Magnesium 24.305															13 Al Aluminum 26.982	14 Si Silicon 28.086	15 P Phosphorus 30.974	16 S Sulfur 32.066	17 Cl Chlorine 35.453	18 Ar Argon 39.948
19 K Potassium 39.098	20 Ca Calcium 40.078	21 Sc Scandium 44.956	22 Ti Titanium 47.867	23 V Vanadium 50.942	24 Cr Chromium 51.996	25 Mn Manganese 54.938	26 Fe Iron 55.845	27 Co Cobalt 58.933	28 Ni Nickel 58.693	29 Cu Copper 63.546	30 Zn Zinc 65.38	31 Ga Gallium 69.723	32 Ge Germanium 72.631	33 As Arsenic 74.922	34 Se Selenium 78.971	35 Br Bromine 79.904	36 Kr Krypton 83.798				
37 Rb Rubidium 85.468	38 Sr Strontium 87.62	39 Y Yttrium 88.906	40 Zr Zirconium 91.224	41 Nb Niobium 92.906	42 Mo Molybdenum 95.95	43 Tc Technetium 98.907	44 Ru Ruthenium 101.07	45 Rh Rhodium 102.906	46 Pd Palladium 106.42	47 Ag Silver 107.868	48 Cd Cadmium 112.414	49 In Indium 114.818	50 Sn Tin 118.711	51 Sb Antimony 121.760	52 Te Tellurium 127.6	53 I Iodine 126.904	54 Xe Xenon 131.294				
55 Cs Cesium 132.905	56 Ba Barium 137.327	57-71		72 Hf Hafnium 178.49	73 Ta Tantalum 180.948	74 W Tungsten 183.84	75 Re Rhenium 186.207	76 Os Osmium 190.23	77 Ir Iridium 192.22	78 Pt Platinum 195.085	79 Au Gold 196.967	80 Hg Mercury 200.592	81 Tl Thallium 204.383	82 Pb Lead 207.2	83 Bi Bismuth 208.980	84 Po Polonium (209)	85 At Astatine (209)	86 Rn Radon (222)			
87 Fr Francium 223.020	88 Ra Radium 226.025	89-103																			
Lanthanide Series																					
57 La Lanthanum 138.905	58 Ce Cerium 140.12	59 Pr Praseodymium 140.908	60 Nd Neodymium 144.24	61 Pm Promethium 144.913	62 Sm Samarium 150.36	63 Eu Europium 151.964	64 Gd Gadolinium 157.25	65 Tb Terbium 158.925	66 Dy Dysprosium 162.50	67 Ho Holmium 164.930	68 Er Erbium 167.259	69 Tm Thulium 168.934	70 Yb Ytterbium 173.055	71 Lu Lutetium 174.967							
Actinide Series																					
89 Ac Actinium 227.028	90 Th Thorium 232.038	91 Pa Protactinium 231.036	92 U Uranium 238.029	93 Np Neptunium 237.048	94 Pu Plutonium 244.064	95 Am Americium 243.061	96 Cm Curium 247.070	97 Bk Berkelium 247.070	98 Cf Californium 251.080	99 Es Einsteinium (254)	100 Fm Fermium 257.095	101 Md Mendelevium 258.1	102 No Nobelium 259.101	103 Lr Lawrencium (262)							

Marco Medves, Giovanna Fronzoni, Mauro Stener; “Optimization of density fitting auxiliary slater type basis functions for time dependent density functional theory”; Journal of Computational Chemistry; 43 (2022) ; 1923–1935

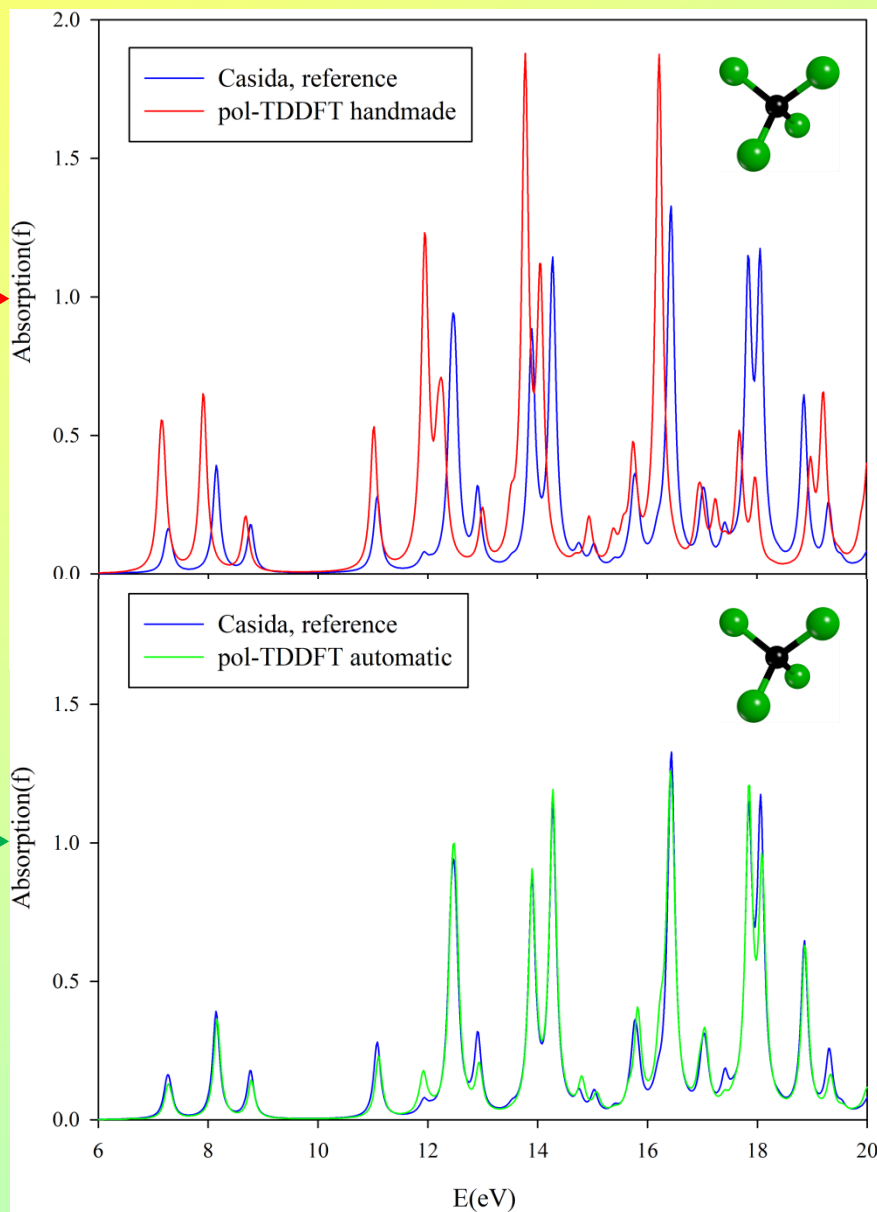
Density fitting basis

Frozen core Cl.2p TZP ZORA, 26 functions

1S	$\alpha=29.10$
2S	$\alpha=29.57$
2S	$\alpha=18.51$
3S	$\alpha=17.08$
3S	$\alpha=11.50$
4S	$\alpha=10.27$
4S	$\alpha=7.25$
4S	$\alpha=5.12$
5S	$\alpha=4.51$
5S	$\alpha=3.29$
5S	$\alpha=2.40$
2P	$\alpha=21.25$
3P	$\alpha=16.90$
4P	$\alpha=13.28$
4P	$\alpha=8.31$
5P	$\alpha=6.53$
5P	$\alpha=4.28$
5P	$\alpha=2.80$
3D	$\alpha=16.31$
4D	$\alpha=12.49$
4D	$\alpha=7.62$
5D	$\alpha=5.86$
5D	$\alpha=3.75$
5D	$\alpha=2.40$
4F	$\alpha=5.00$
4F	$\alpha=3.00$
5G	$\alpha=3.50$

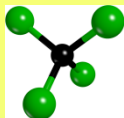
Random handmade

Automatic trajectory

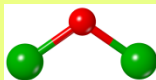


Descriptors: match with respect to Casida reference

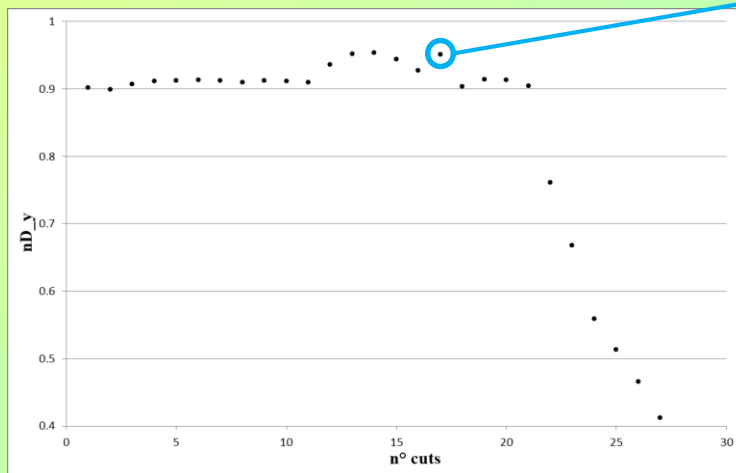
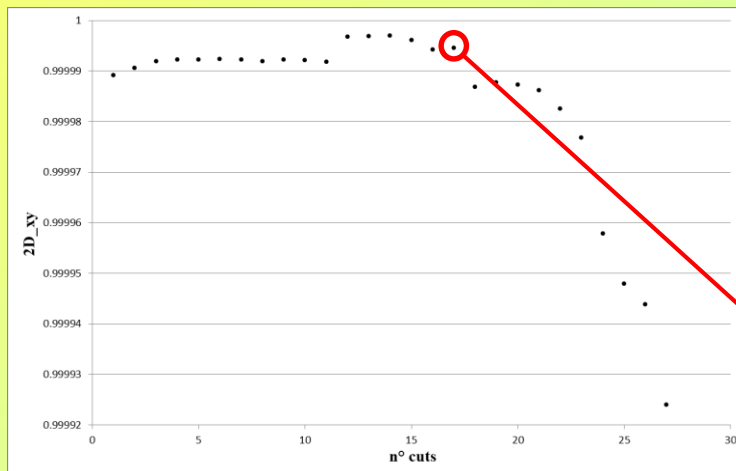
CCl_4



Cl_2O



HCl

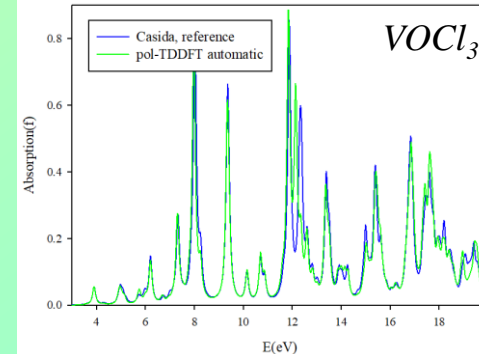
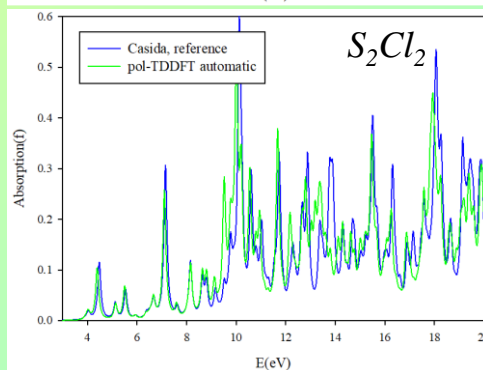
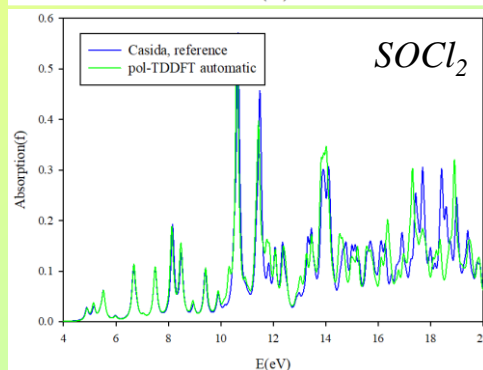
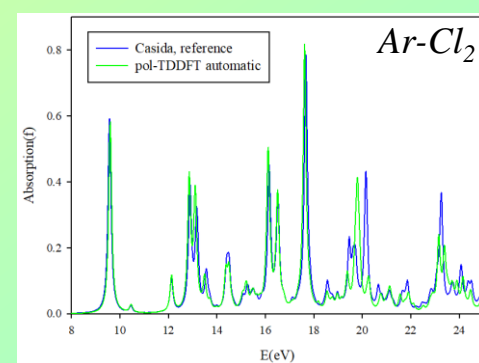
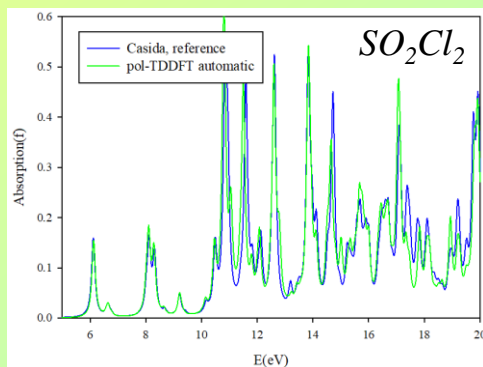
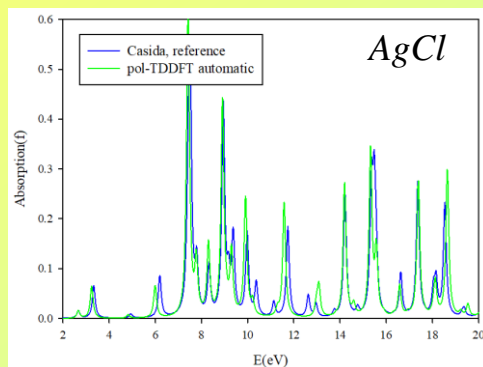
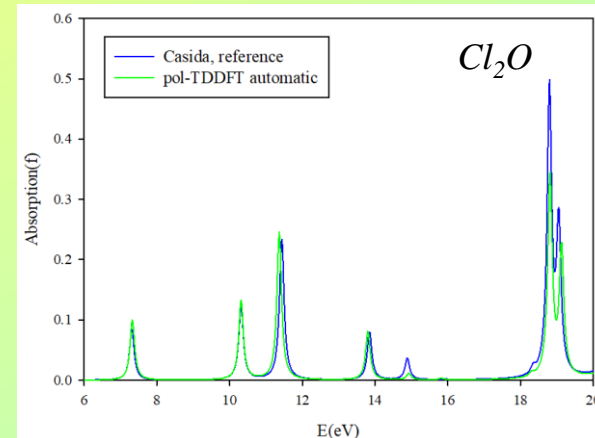
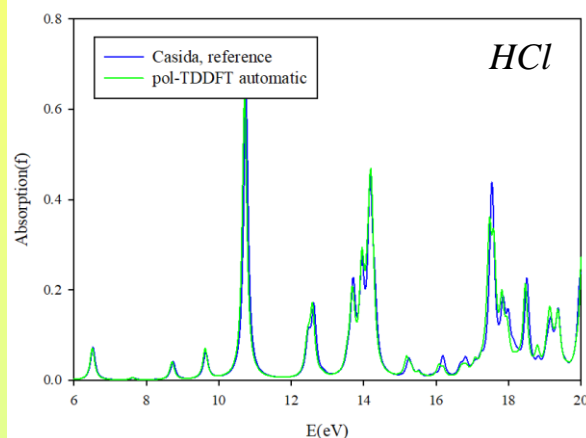
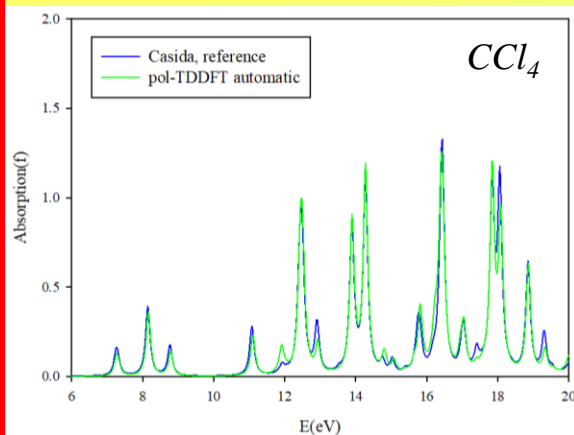


Result

4S	$\alpha=5.12$
5S	$\alpha=4.51$
5S	$\alpha=3.29$
5S	$\alpha=2.40$
4P	$\alpha=8.31$
5P	$\alpha=4.28$
5P	$\alpha=2.80$
5D	$\alpha=3.75$
5D	$\alpha=2.40$
4F	$\alpha=5.00$
4F	$\alpha=3.00$

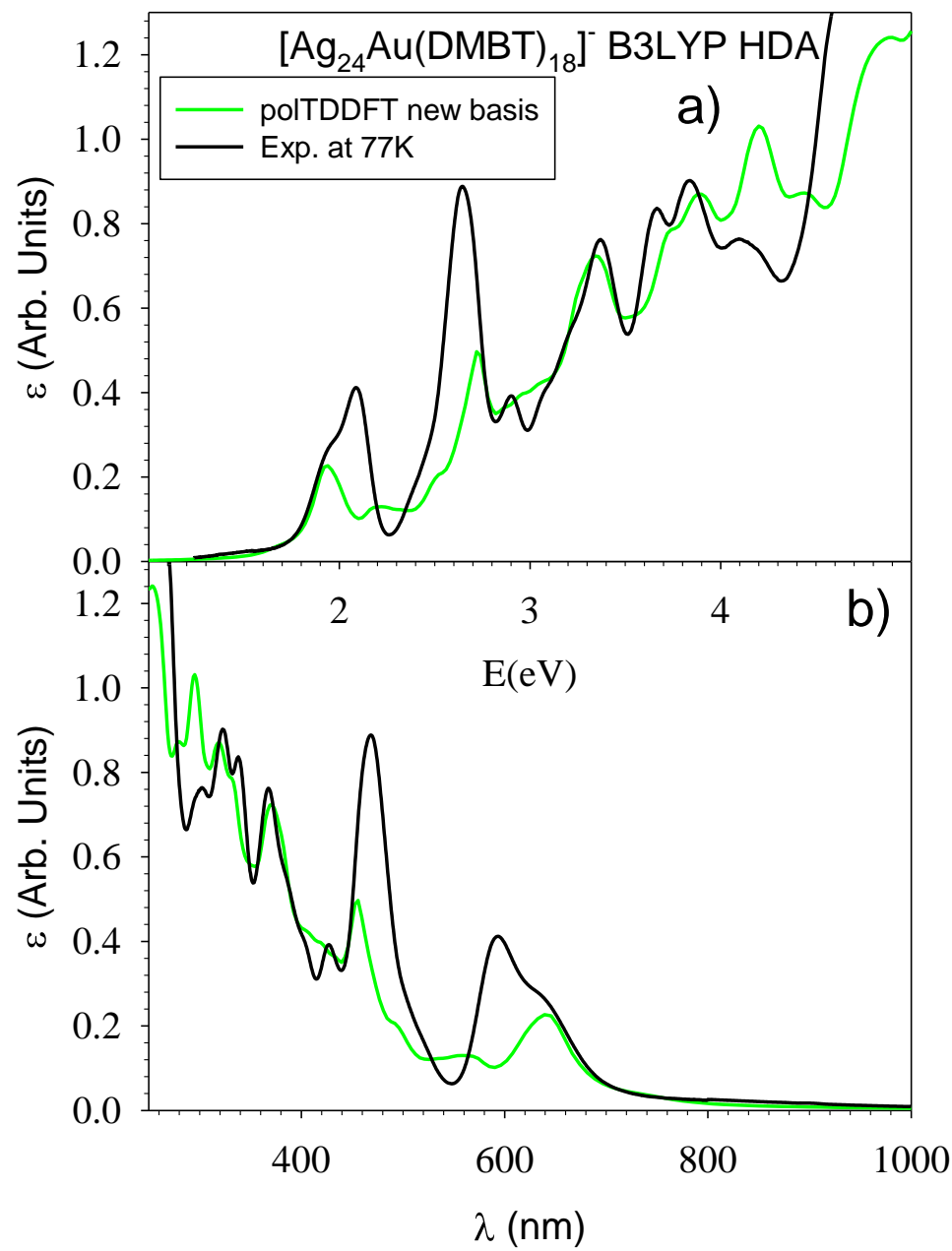
Results and testing

Inside the collection



Outside the collection

Applications: $[\text{Ag}_{24}\text{Au}(\text{DMBT})_{18}]^-$ exp. at 77 K



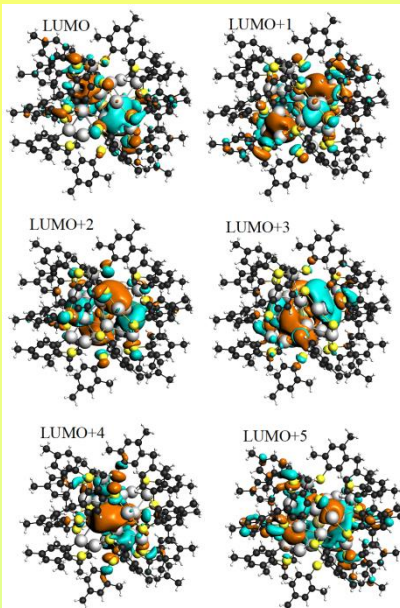
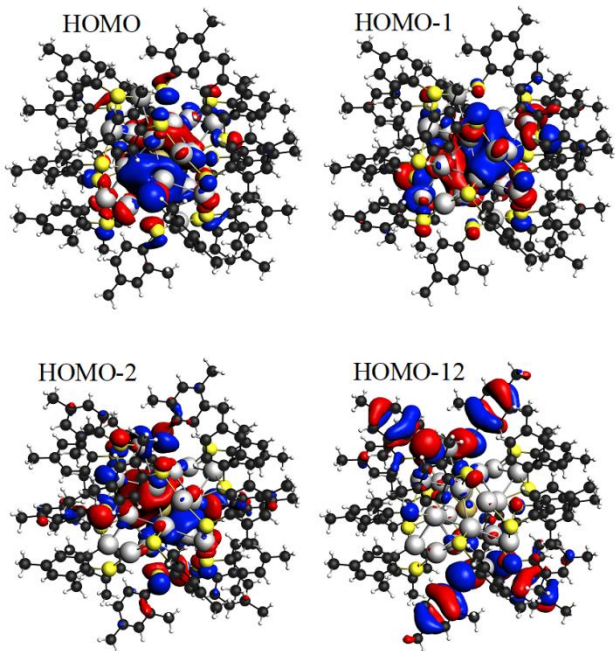
The photoabsorption data registered at 77K from the group of F. Maran in Padua.

In the low T spectrum emerge new features not visible at RT in excellent agreement with theory.

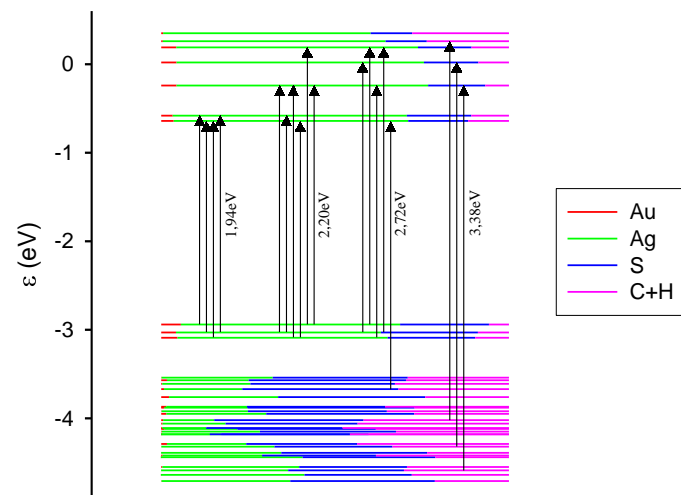
M. Medves, L. Sementa, D. Toffoli, G. Fronzoni, K. R. Krishnadas, F. Maran, T. Bürgi, A. Fortunelli, and M. Stener

“Predictive optical photoabsorption of $[\text{Ag}_{24}\text{Au}(\text{DMBT})_{18}]^-$ via efficient TDDFT simulations”

J. Chem. Phys. 155 (2021) 084103



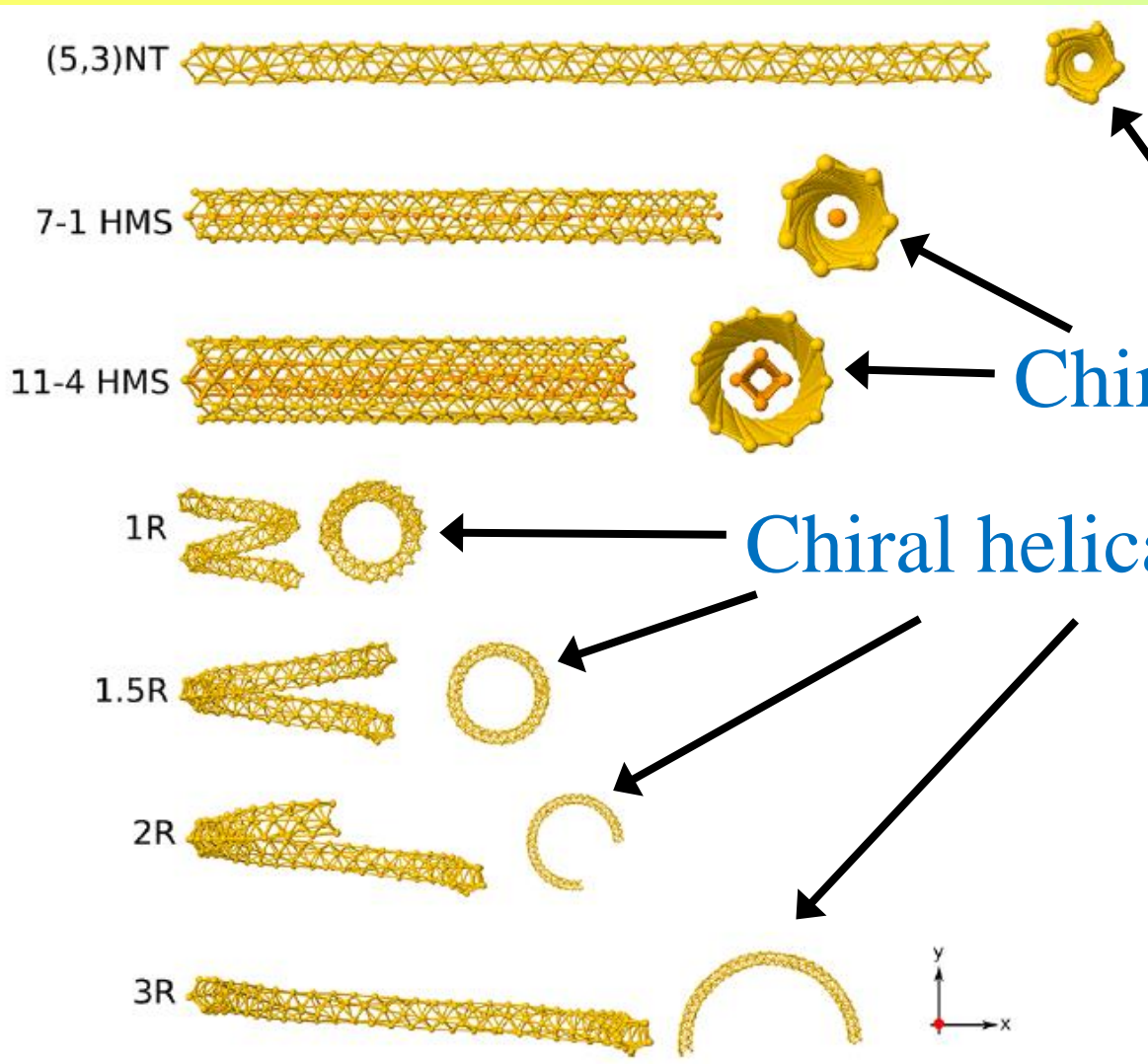
Inability of non-hybrid xc to describe the balance between metal and sulfur contributions. Tendency to move bands around the HOMO-LUMO gap to too low energies, thus underestimating the position of the corresponding excitations. Such excitations are blue-shifted and merged with higher-energy peaks when hybrid xc-functionals are employed



Transition energy (eV)	f	Assignment (only contribution > 10%)
1.94	0.23	21.7% HOMO (28% Ag 4s, 18% S 3p, 10% Ag 4p) \rightarrow LUMO+1 (34% Ag 4s, 18% Ag 4p, 11% S 3p) 17.9 % HOMO-1 (27% Ag 4s, 20% S 3p) \rightarrow LUMO (31% Ag 4s, 19% Ag 4p) 17.3% HOMO-2 (28% Ag 4s, 19% S 3p) \rightarrow LUMO 16.7% HOMO-1 \rightarrow LUMO+1
2.20	0.13	34.7% HOMO-1 \rightarrow LUMO+2 (28% Ag 4p, 26% Ag 4s)
2.72	0.50	19.9% HOMO-1 \rightarrow LUMO+3 (27% Ag 4s, 24% Ag 4p, 10% S 3p) 16.3% HOMO \rightarrow LUMO+4 (25% Ag 4s, 24% Ag 4p)
3.38	0.72	11.5% HOMO-12 (37% S 3p, 18% C 2p) \rightarrow LUMO+5 (31% Ag 4p)

Circularly Polarized Plasmons in Chiral Gold Nanowires via Quantum-Mechanical Design

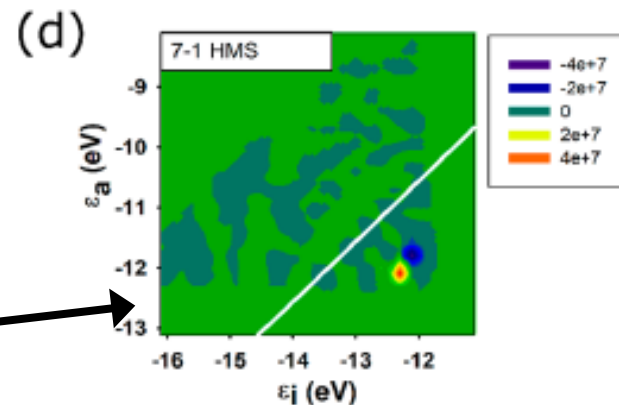
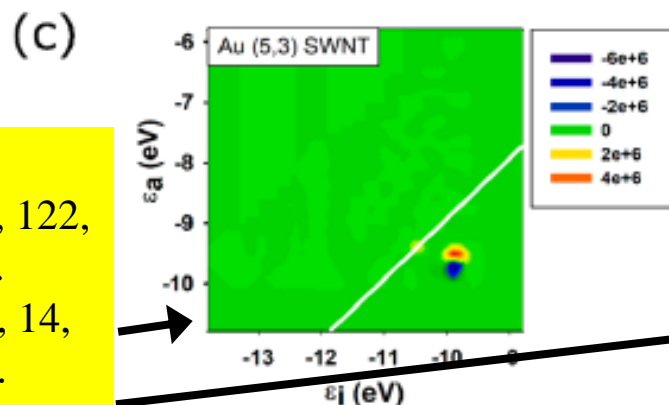
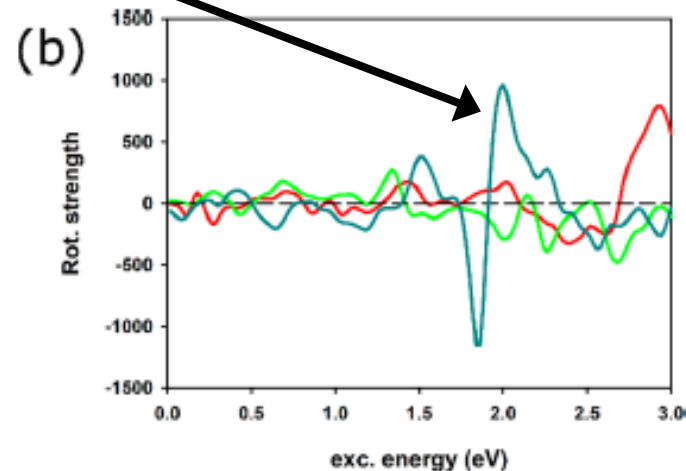
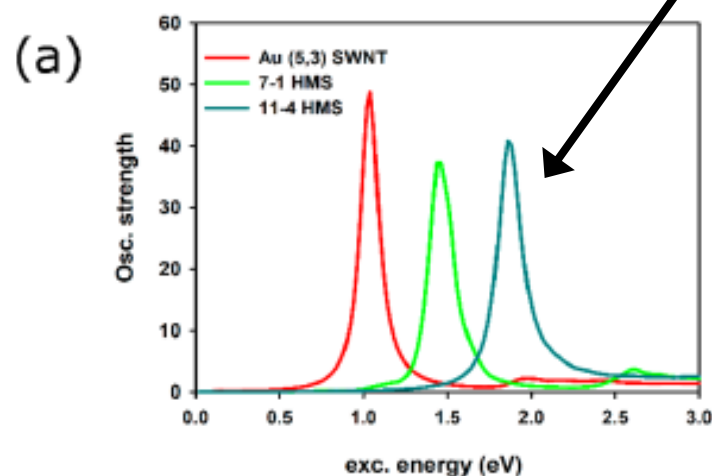
D. Toffoli, A. Russi, G. Fronzoni, E. Coccia, M. Stener, L. Sementa and A. Fortunelli, *J. Phys. Chem. Letters* 2021, **12**, 5829.



Chiral linear nanowires

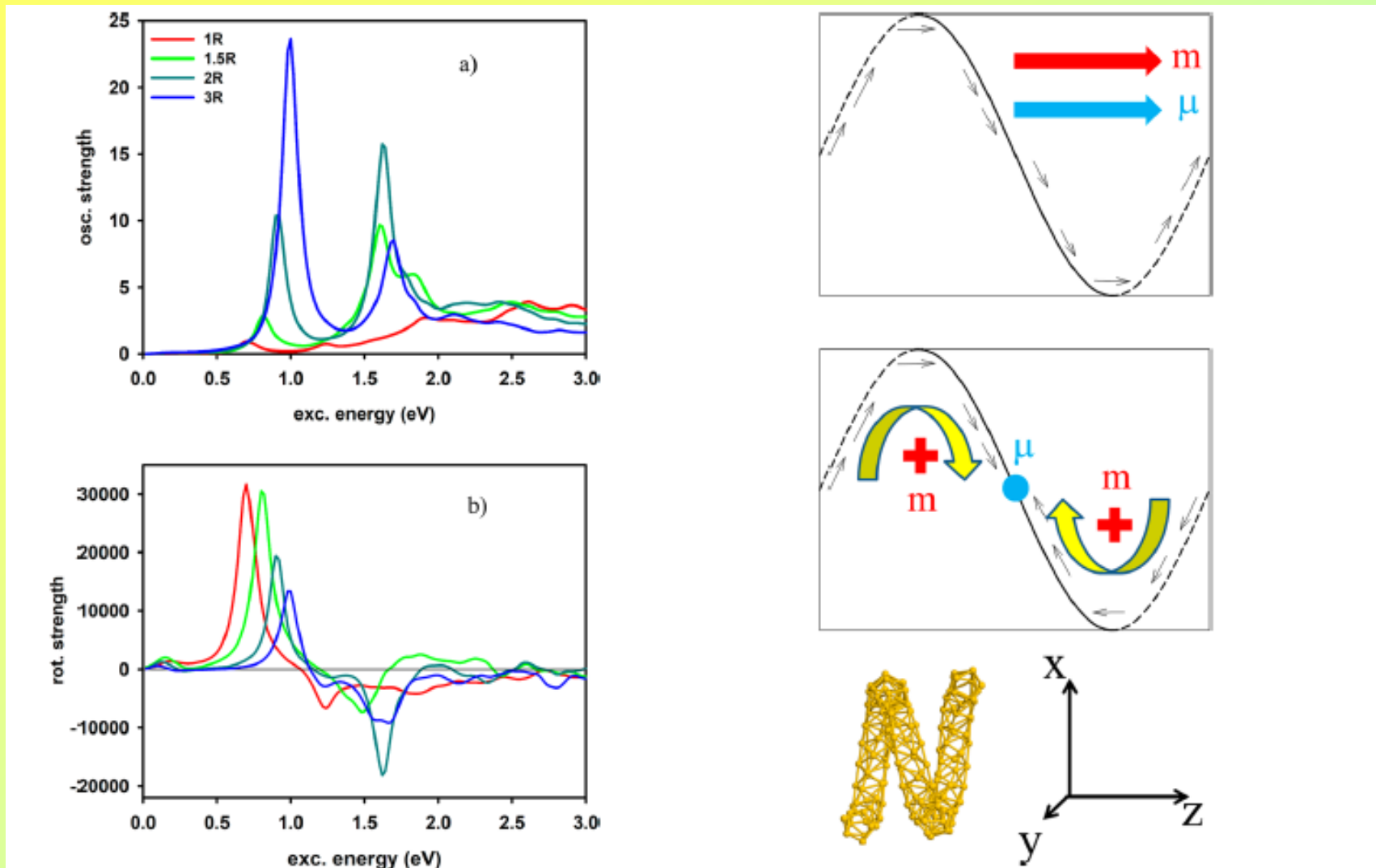
Chiral helical (coiled) nanowires

Low Dichroism Plasmons for linear chiral nanowires, emerging in 11-4



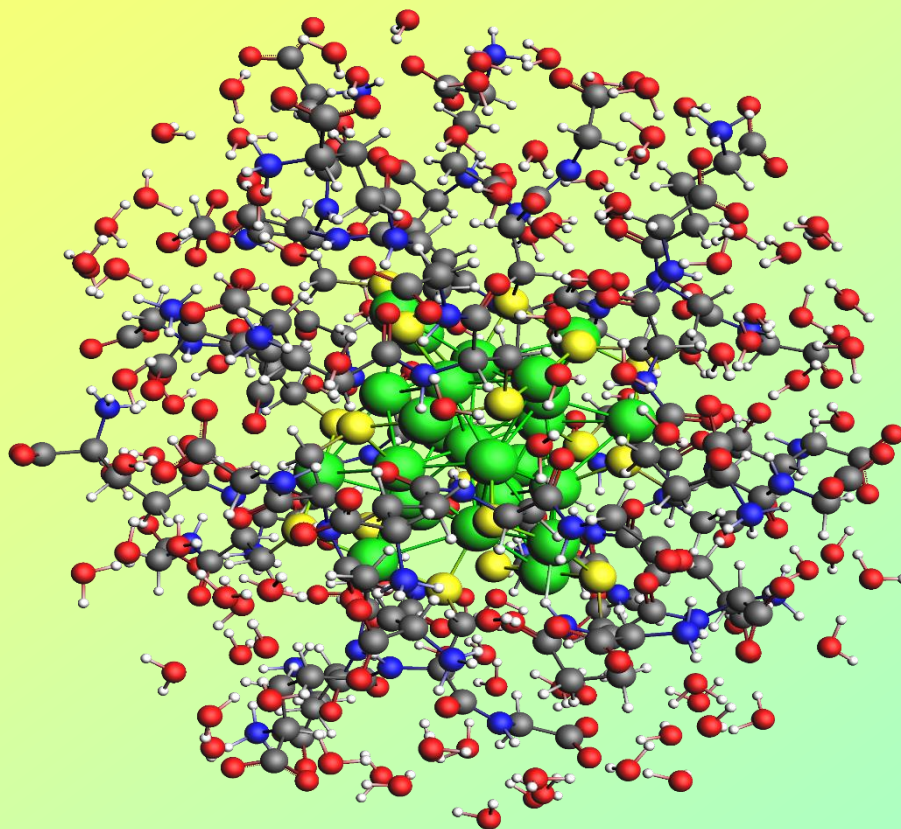
ICM plots:
JPCC 2018, 122,
4524–4531.
JCTC 2018, 14,
3703–3714.

Very large dichroism in plasmons for helical (coiled) chiral nanowires!



Longitudinal and transversal plasmons with opposite dichroism

Largest system considered so far: 1068 atoms, no symmetry, explicit solvent: $[Au_{25}(GSH)_{18}]^{-1}-(H_2O)_{126}$



•Inclusion by MD and ED of conformational degrees of freedom for the calculations of ECD of chiral clusters

Marta Monti (HPC Europa3): Ongoing collaboration with S. Corni (Padua), M. Aschi (L'Aquila) and H. Hakkinen (Jyvaskyla)

Other applications

- Calculation of transition moments between excited states and Real Time TDDFT

P. Grobas-Illobre, M. Marsili, S. Corni, M. Stener, D. Toffoli and E. Coccia

J. Chem. Theo. Comput. 17 (2021) 6314-6329

- Chiral functionalization of an atomically precise noble metal cluster: Insights into the origin of chirality and photoluminescence

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- Inclusion by MD and ED of conformational degrees of freedom for the calculations of ECD of chiral clusters

Marta Monti (HPC Europa3): Ongoing collaboration with S. Corni (Padua), M. Aschi (L'Aquila) and H. Hakkinen (Jyvaskyla)

- More efficient HDA with Resolution of Identity (RI)

Pierpaolo D'Antoni (HPC Europa3): Ongoing collaboration with L. Vissker (Amsterdam)

- Effect of O adsorption on optical (plasmon) properties of silver clusters

Elena Zerbato (HPC Europa3): Ongoing collaboration with K. Neyman (Barcelona)

\$AMSBIN/ams << eor

polTDDFT input for AMS

ENGINE RESTART au170_scf_z2.t21

SYSTEM #1

Atoms

Au 2.786100 0.000000 -30.115689

(...)

End

Charge 2.0

END #1

TASK SINGLEPOINT #2

ENGINE ADF #3

Relativity

Formalism ZORA

Level scalar

End

Basis

PerAtomType Symbol=Au File=\$AMSRESOURCES/ADF/POLTDDFT/TZP/Au.4f

End

(...)

polTDDFT input for AMS

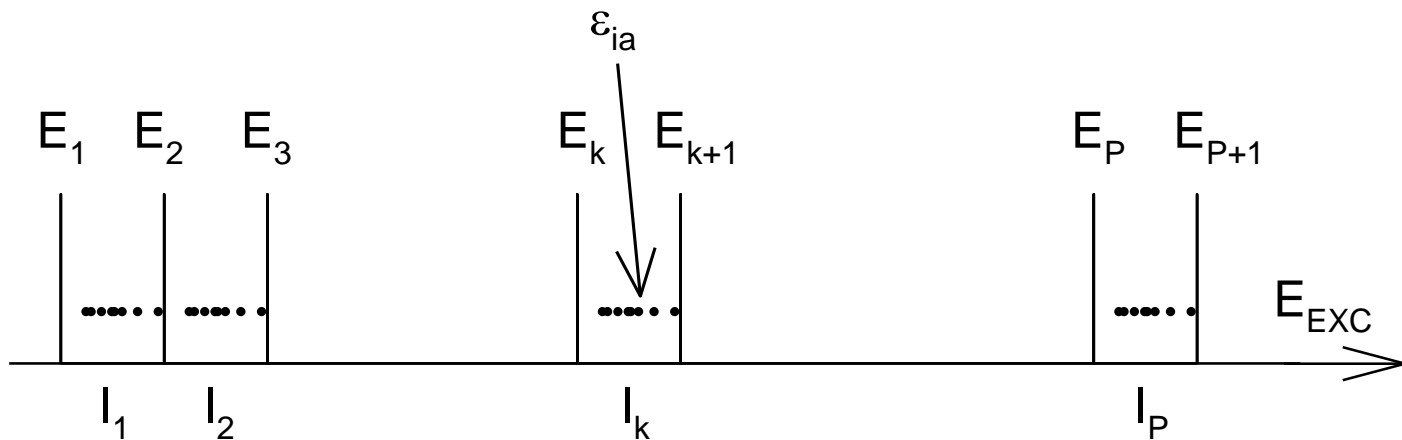


Fig. 2

(...)

Poltdfft

FreqRange 0.02 5.02

NFreq 249

KGrid 8.

NGrid 320

Lifetime 0.060

Cutoff 3.

End

(...)

the spectrum is calculated from 0.0 to 5 eV

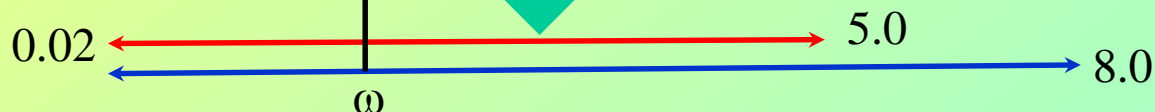
249 points (step = $(5.00 - 0.02)/249 = 0.02$ eV)

the excitations are calculated up to 8 eV (E_P)

320 I_k (width = $8/320 = 0.025$ eV)

imaginary photon energy (eV) = HWHM Lorentzian broadening

excitations are included up to $\omega + \text{cutoff}$



Cutoff: default 4 eV good for large systems, for small/medium systems cutoff may be increased up to 20 eV

Recommendation: check cutoff choice wrt a Casida calculation of the lowest part of the spectrum

Conclusions:

- The density-matrix **Casida** approach is **not practical to treat big metal clusters**, since many roots (lowest eigenvalues) are necessary.
- The complex polarizability **polTDDFT** algorithm is proposed to treat large systems
- **Implementation** of the complex polarizability algorithm is completed in **AMS2021** code and published: JCP 143 (2015) 024106.
- **Hybrid XC** are the best choice in terms of agreement with experiment. But very demanding, **HDA** solves the problem (AMS2021)
- The **density fitting basis** set has been extended and reoptimized (**AMS2021**)
- All such new features are already available in AMS2022.
- The suggested protocol has proven predictive for alloyed MPC, further comparison with low T spectra for other systems will be necessary to confirm this conclusion in general.
- **Further extensions**: AMS2023: polTDDFT fast HDA RI, unrestricted HDA Casida, restarts options, ICM in GUI. AMS2024: unrestricted polTDDFT, RS functionals with RI in polTDDFT, improve parallelization.

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Thank you for your attention!