



Research fields in TCCM Partner Trieste University (UTS)

If several groups and/or institutes/departments exist please enter the acronyms and identify group leader(s) in next lines

Institute/Department (if different exists)	Acronym	Group Leaders	Web Page	
Dipartimento di Scienze Chimiche e Farmaceutiche (DSCF)	THEOCHEM	Stener, Fronzoni, Toffoli, Coccia	under construction (ready end of July 2021)	
METHODOLOGY				
General keyword	Details in topic	Researchers involved	Institute (Group Acronym)	

DFT and TDDFT	Development of TDDFT algorithms for optical properties of large systems	Mauro Stener	THEOCHEM	
	Development of DFT methods for core electron spectroscopies	Giovanna Fronzoni		
	Development of methods for vibronic coupling	Daniele Toffoli	THEOCHEM	
	Development of time-domain methods for electron dynamics and quantum coherence in ultrafast spectroscopies	Emanuele Coccia		
			THEOCHEM	
Quantum Monte Carlo (QMC)	Excited-state properties using linear-response QMC	Emanuele Coccia	THEOCHEM	
Atomic and Molecular Photoionization	Ab-initio determination of molecular excited states	Daniele Toffoli, Mauro Stener		
Ab-initio	Core excited states via multireference methods	Daniele Toffoli, Giovanna Fronzoni		

Artificial Intelligence	Automatic generation of density fitting and mapping of Potential Energy Surface	Daniele Toffoli, Giovanna Fronzoni, Mauro Stener	THEOCHEM	
APPLICATIONS				
Systems	Property	Methods	Researchers involved	Insitiute (Group Acronym)
Metal clusters	Plasmon resonance	TDDFT	Stener, Fronzoni, Toffoli, Coccia	THEOCHEM
Monolayer protected clusters	Circular Dichroism		Stener, Fronzoni, Toffoli, Coccia	THEOCHEM
Gas-phase molecules /molecules with nanoparticle	High-harmonic generation, decoherence, absorption	ab initio, TDDFT, QMC	Coccia	THEOCHEM
Adsorbed molecules	Core-electron theoretical Spectroscopy (NEXAFS, XPS)	DFT, TDDFT, ab-initio	Fronzoni, Toffoli, Stener	THEOCHEM
Gas phase molecule				