

COST 'Our Astrochemical History' Action CM1401

MPE 'CAS@MPE'

CNRS 'Interfaces des Physiques Numérique et Théorique'

MIAPP, Garching

Theory of Gas Phase Scattering and Reactivity for Astrophysics

Extended workshop

Garching, MIAPP

23 November – 8 December 2015

Colloquium on kinetics and scattering theory for astrophysics

Garching, MPE seminar room

26 November – 27 November

Scientific program Colloquium

Wednesday, 25-11

25-11	17:30	Welcome, registration, refreshments, MIAPP		
	18:30	COST, CAS@MPE	Laurent Wiesenfeld Paola Caselli	

Thursday, 26-11

26-11	9:00	Welcome, MPE <i>New Seminar Room 1.1.18b (downstairs)</i>		
	9:30	Introduction	Motivation of this workshop	Laurent Wiesenfeld Paola Caselli
26-11	10:00	Session 1	Astronomy	Chair: Bo Zhao
	10:00-10:30		Molecular complexity in star forming regions: What we know and what we do not.	Cecilia Ceccarelli
	10:30-11:00		Some Poorly Understood Classes of Interstellar Reactions.	Eric Herbst
	11:00	<i>Coffee</i>	<i>MPE</i>	
26-11	11:30	Session 2	Models / Chemistry	Chair: Seyit Höcük
	11:30-12:00		Impact of collisional and chemical rates on astrochemistry modelling in protoplanetary disks	Wing-Fai Thi
	12:00-12:30		Revisiting gas-phase chemistry in astrochemical models	Nadia Balucani
	12:30-12:45		KIDA (Kinetic database for Astrochemistry): Present and Future	Liton Majundar
26-11	13:00	Lunch	Canteen	
26-11	14:30	Session 3	Theoretical chemistry, PES	Chair: Alan Heays
	14:30-15:00		Ab initio study of small molecules PES : 2 case studies	Denis Duflot
	15:00-15:30		Potential Energy Surfaces for reaction dynamics	João Brandão
	15:30-16:00		Ab initio modeling of surface-induced reactions of astrochemical interest. Strategies and current limitations	Alberto Rimola
	16:00	<i>Coffee</i>	<i>MPE</i>	
	16:30	Session 4	Theoretical chemistry, spectroscopy	Chair: Michela Giuliano
	16:30-		Rotational spectroscopy as a tool to investigate molecules in space	Cristina Puzzarini

	17:00			
	17:00-17:30		Rotational Spectroscopy and Pressure Broadening of Astrophysical Ions	Luca Bizzocchi
	17:30-18:00		Molecules in Motion	Attila Czászár
	18:00	End of day		
	19:30	Dinner, Rondell Restaurant, Garching		

Friday, 27-11, MPE New Seminar Room 1.1.18b (downstairs)				
27-11	9:30	Session 5	Quantum scattering / reactivity	Chair: Thanja Lamberts
	9:30-10:00		From scattering resonances to rate coefficients for astrophysical modeling	Ad van der Avoird
	10:00-10:30		A Priori Kinetics: Coupling Electronic Structure Theory with Statistics, Dynamics, and the Master Equation	Stephen Klippenstein
	10:30-11:00		Quantum scattering calculations: Closing the gap between observations and astrochemical models	François Lique
	11:00-11:15		Quantum mechanical calculation of the collision-induced absorption spectra of N ₂ and O ₂	Tijs Karman
	11:20	Coffee	MPE	
	11:50	Session 6	Classical dynamics / dynamical systems	Chair: Jake Laas
	11:50-12:20		Phase Space geometry and Chemical Reaction Dynamics: Past, Present, and Future	T. Komatsuzaki
	12:20-12:50		Dynamical Reaction theory : Beyond the conventional statistical reaction theory	M. Toda
27-11	13:00	Lunch	Canteen	
	11:50-12:20		Quantum Transition State Theory	H. Waalkens
	15:00-15:30		Classical approach to energy transfer: successes and limitations	A. Faure
	15:30-16:00		Dynamical Reaction Theory: Beyond the conventional perturbation theory	H. Teramoto
	16:00	Coffee	MPE	
	16:30	Session 7	Time-dependent/Semi-classics	Chair: Anton Vasyunin
	16:30		MCTDH (<i>provisional title</i>)	F. Gatti
	17:00		Recent advances in the mixed quantum/classical theory of inelastic scattering	D. Babikov
	17:30		Closing of the Colloquium	
	17:30		Presentation of week 2; White paper. Open discussion	L. Wiesenfeld, Paola Caselli
	18:30		Farewell	

Scientific program Extended Workshop

Monday-Wednesday	Date	Workshop	MIAPP Offices
Monday	23-11	Classical dynamics : State of the art	Komatsuzaki, Terao
<i>Coffee at MIAPP, lunch at canteen</i>			
Tuesday	24-11	Chemical networks, as seen by dynamical system theory	Komatsuzaki, WF Thi, P. Caselli
<i>Coffee at MIAPP, lunch at canteen</i>			
Wednesday	25-11	Potential energy surfaces Current problems in astrochemistry	J Brandão, D. Duflot E. Herbst
<i>Coffee at MIAPP, lunch at canteen</i>			
Wine and cheese	17:30	MIAPP	
Thursday-Friday	26-11/ 27-11	Colloquium	MPE Conference room
<i>Coffee at MIAPP, lunch at canteen</i>			
Monday-Friday	30-11/4-12	Workshop	MIAPP Offices
Monday	30-11	Transition state theory	S. Klippenstein, M. Toda, H. Waalkens
<i>Coffee at MIAPP, lunch at canteen</i>			
Tuesday	01-12	Quantum dynamics	Ad van der Avoird, D Skouteris
<i>Coffee at MIAPP, lunch at canteen</i>			
Wednesday	02-12	Trajectories & tunneling	O. Roncero
<i>Coffee at MIAPP, lunch at canteen</i>			
Thursday	03-12	Semi-classics	A. Semenov or TBD
<i>Coffee at MIAPP, lunch at canteen</i>			
Friday	04-12	Spectroscopy and dynamics	L. Bizzochi, L. Wiesenfeld
<i>Coffee at MIAPP, lunch at canteen</i>			
Monday-Tuesday	7-12/8-12	Workshop	MIAPP Offices
Monday-Tuesday		Classical dynamics and semi-classical dynamics advances & exploration	A. Semenov, M. Toda, LW + all still present Going beyond today's possibilities !

			White paper writing
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