

**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***

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**Extended workshop**

*Garching, MIAPP*

*23 November – 8 December 2015*

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**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	<b>Session 1</b>	<b>Astronomy</b>	<b>Chair: Bo Zhao</b>
	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	<b>Session 2</b>	<b>Models / Chemistry</b>	<b>Chair: Seyit Höcük</b>
	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	<b>Lunch</b>	<b>Canteen</b>	
26-11	14:30	<b>Session 3</b>	<b>Theoretical chemistry, PES</b>	<b>Chair: Alan Heays</b>
	14:30-15:00		Ab initio study of small molecules PES : 2 case studies	Denis Dufлот
	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	<b>Session 4</b>	<b>Theoretical chemistry, spectroscopy</b>	<b>Chair: Michela Giuliano</b>
	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
	<b>18:00</b>	<b>End of day</b>		
	<b>19:30</b>	<b>Dinner, Rondell Restaurant, Garching</b>		

<b>Friday, 27-11, MPE</b> New Seminar Room 1.1.18b (downstairs)				
<b>27-11</b>	<b>9:30</b>	<b>Session 5</b>	<b>Quantum scattering / reactivity</b>	<b>Chair: Thanja Lamberts</b>
	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 <sub>2</sub> and O <sub>2</sub>	Tijs Karman
	<b>11:20</b>	<b>Coffee</b>	<b>MPE</b>	
	<b>11:50</b>	<b>Session 6</b>	<b>Classical dynamics / dynamical systems</b>	<b>Chair: Jake Laas</b>
	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
<b>27-11</b>	<b>13:00</b>	<b>Lunch</b>	<b>Canteen</b>	
	14:30-15:00		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
	<b>16:00</b>	<b>Coffee</b>	<b>MPE</b>	
	<b>16:30</b>	<b>Session 7</b>	<b>Time-dependent/Semi-classics</b>	<b>Chair: Anton Vasyunin</b>
	16:30		MCTDH ( <i>provisional title</i> )	F. Gatti
	17:00		Recent advances in the mixed quantum/classical theory of inelastic scattering	D. Babikov
	<b>17:30</b>		<b>Closing of the Colloquium</b>	
	17:30		Presentation of week 2; White paper. Open discussion	L. Wiesenfeld, Paola Caselli, A.Faure
	<b>18:30</b>		<b>Farewell</b>	

## Scientific program

### Extended Workshop

<b>Monday-Wednesday</b>	<b>Date</b>	<b>Workshop</b>	<b>MIAPP Offices</b>
Monday	23-11	Classical dynamics : State of the art	Komatsuzaki, Terao
<b>Coffee at MIAPP, lunch at canteen</b>			
Tuesday	24-11	Chemical networks, as seen by dynamical system theory	Komatsuzaki, WF Thi, P. Caselli
<b>Coffee at MIAPP, lunch at canteen</b>			
Wednesday	25-11	Potential energy surfaces Current problems in astrochemistry	J Brandão, D. Duflot E. Herbst
<b>Coffee at MIAPP, lunch at canteen, 13:00</b>			
<b>Wine and cheese</b>	<b>17:30</b>	<b>MIAPP</b>	
<b>Thursday-Friday</b>	<b>26-11/ 27-11</b>	<b>Colloquium</b>	<b>MPE Conference room</b>
<b>Monday-Friday</b>	<b>30-11/4-12</b>	<b>Workshop</b>	<b>MIAPP Offices</b>
Monday	30-11	Transition state theory	S. Klippenstein, M. Toda, H. Waalkens
<b>Coffee at MIAPP, lunch at canteen</b>			
Tuesday	01-12	Quantum dynamics	Ad van der Avoird, D Skouteris
<b>Coffee at MIAPP, lunch at canteen</b>			
Wednesday	02-12	Trajectories & tunneling	O. Roncero
<b>Coffee at MIAPP, lunch at canteen</b>			
Thursday	03-12	Semi-classics	A. Semenov or TBD
<b>Coffee at MIAPP, lunch at canteen</b>			
Friday	04-12	Spectroscopy and dynamics	L. Bizzochi, L. Wiesenfeld
<b>Coffee at MIAPP, lunch at canteen</b>			
<b>Monday-Tuesday</b>	<b>7-12/8-12</b>	<b>Workshop</b>	<b>MIAPP Offices</b>