Book of abstracts
DEEP-GAS 2022

COST Action CA18212
MD-GAS
Molecular Dynamics
in the GAS phase

About MD-GAS

The main aim of the MD-GAS COST Action (CA18212) is to develop a new physical and chemical toolbox to significantly advance the understanding of:
- Gas phase molecular dynamics induced in interactions between molecules or clusters and photons, electrons, or heavy particles.
- Its consequences for a broad range of applications in e.g. astrochemical and atmospheric sciences, and molecular radiation damage.
https://mdgas.eu/
info@mdgas.eu

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Among fundamental atomic and molecular physics, chemical physics, and applications in radiation therapy and -damage on the nanoscale, astrochemistry, astrobiology, atmospheric science, and climate research interests of the working groups 2 and 3, the meeting will host a session specifically focused on systems of biological interest as well as a session fully dedicated to Early Career Investigators, an essential tradition of our MD-GAS meetings!
https://deep-gas.sciencesconf.org/

DEEP-GAS Committee

Sergio Díaz-Tendero (WG 3 Leader)
Paola Bolognesi (WG 2 Leader)
Dariusz G. Piekarski (WG 2 Co-Leader)
Lucas Schwob (WG 2 Co-Leader)
Sylvain Maclot (WG 3 Co-Leader)
Ana Isabel Lozano (WG 3 Co-Leader)
Henning Zettergren (Action Chair)
Alicja Domaracka (Action Vice Chair)

1 Schedule

	Tuesday 4th	Wednesday 5th	Thursday 6th	Friday 7th
09:00	Registration			
09:45	Welcome			
10:00	Raimund Feifel (Chair: Paola Bolognesi)	Rebecca Boll (Chair: Sylvain Maclot)	Lorenzo Avaldi (Chair: Henning Zettergren)	Patrick Španěl (Chair: Rita Prosmiti)
10:45	Coffee break	Coffee break	Coffee break	Coffee break
11:15	Chair: Cristina Sanz-Sanz	Chair: Alicia Palacios	Chair: Lucas Schwob	Chair: Sergio Díaz-Tendero
	Vincent Wanie	Laura Rego	Marc Simon	Mathieu Gisselbrecht
11:45	Janina Kopyra	Eva Muchova	Teodora Kirova	Yoni Toker
12:15	João Ameixa	Rocío Borrego	Aleksandar Milosavljević	Károly Tőkési
12:45	Francisco Fernández-Villora	Eva Vos	Juliette Leroux	Nicolina Pop
13:05	**LUNCH**	**LUNCH**	**LUNCH**	**LUNCH**
14:30	Chair: Ana Lozano	Chair: Marta Łabuda	Chair: Wojciech Gawelda	
	Mathias Poline	Felix Iacob	Ori Licht	
14:50	Carlos Guerra	Demeter Tzeli	Branislav Milovanović	
15:10	Bart Oostenrijk	Vincenzo Laporta	Dariusz Kedziera	
15:30	Olga Lushchikova	Oded Heber	Sándor Demes	
15:50		Poster Session + TAPAS served		
16:00	Coffee break		Coffee break	
16:30	Chair: Darek Piekarski		Chair: Ewa Erdmann	
	Patrik Hedvall		Arno Ehresmann	
17:00	Fábris Kossoski		Judit Montes de Oca	
17:20	Jacopo Chiaranelli		Jelena Maljkovic	
17:40	Josef Filgas			
18:00	Daniel González		Roof Top Evening	
18:20				

Chair: Wojciech Gawelda

14:30 - 14:50	Ori Licht, Department of Physics and the Institute of Nanotechnology, Bar-Ilan University - *Bond formation within amino acids clusters following irradiation by UV light*
14:50 - 15:10	Branislav Milovanović, Faculty of Physical Chemistry, University of Belgrade - *Formation of Cyclobutane Dimers from the Solvated Uracil Stacks*
15:10 - 15:30	Dariusz Kedziera, Faculty of Chemistry, Nicolaus Copernicus University - *Towards an effective description of hydrogen-bonded systems – modification of the hydrogen basis set*
15:30 - 16:00	Sándor Demes, Univ Rennes, CNRS, IPR (Institut de Physique de Rennes) *Recent advances in collisional excitation of interstellar polyatomic molecules*
16:00 - 16:30	Coffee break

Chair: Ewa Erdmann

16:30 - 17:00	Arno Ehresmann, Institute of Physics, University of Kassel - *Energy and charge transfer processes in clusters investigated by photon and multi-coincidence spectroscopies*
17:00 - 17:20	Judit Montes de Oca, Institute of Fundamental Physics, IFF-CSIC - *New kernel-based machine-learning potential energy surfaces for spectroscopic characterization of Ng-containing molecules: the case of* $[Ar_2H]^+$
17:20 - 17:40	Jelena Maljkovic, Institute of Physics, University of Belgrade *Elastic electron scattering on the aneasthetic molecules in the gas phase*
18:00 - 22:00	Roof top evening

Elastic electron scattering on the aneasthetic molecules in the gas phase

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We have investigated elastic electron scattering cross sections from anesthetics molecules in the gas phase for intermediate impact energies. Measurements of the elastic differential cross sections (DCS) have been performed with a crossed electron-target beam apparatus UGRA [1], settled at the Institute of Physics in Belgrade. Relative DCSs were put on an absolute scale by using the relative flow technique [2]. Calculations are based on Independent Atom Model (IAM) by using the screening corrected additivity rule (SCAR) technique and including interference effects. Measurements have been carried out for anesthetics molecules, such as sevoflurane [1] and halothane. Absolute DCSs for elastic electron scattering from halothane at 200, 250, and 300 eV are presented in Figure 1.

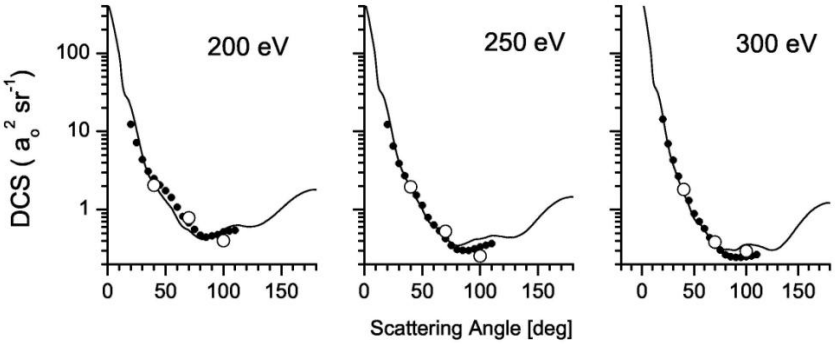

Figure 1: Angular dependence of the DCSs for elastic electron scattering from halothane at 200, 250 and 300 eV. Circles represent absolute experimental differential cross sections; open circles represent absolute values obtained by relative flow method and solid lines represent calculations.

Acknowledgements

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References

[1] J. Vukalović, J.B.Maljković., F. Blanco, G. García, B. Predojević and B .P. Marinković., *Int. J. Mol. Sci.* **23,** 10021 (2022).

[2] J. C.Nickel, P. V. Zetner., G. Shen, and S. Trajmar, *J. Phys. E :Sci. Instrum*., **22**,730, (1989).