



SEMINAR

8th July 2021 - 10:00 h Zoom virtual meeting

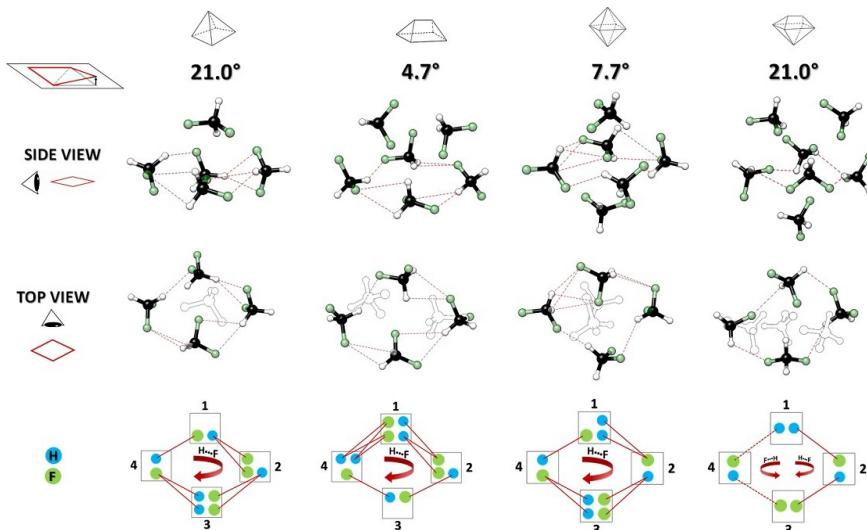
<https://desy.zoom.us/j/91202137161> (Meeting-ID: 912 0213 7161, Password: 845021)

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Decoding (bio)structures and applications through high-resolution spectroscopy: Microwave and laser spectroscopies

I present several studies on biomolecules (carbohydrates and glycopeptides) and several applications, exploiting an experimental strategy which combines microwave and laser spectroscopies in high resolution, NMR, computation and synthesis. Laser spectroscopy offers high sensitivity and selectivity, making it ideal for studying biochemical systems of medium-large size [1,2]. Moreover, microwave spectroscopy provides higher resolution and direct access to molecular structure [3,4]. This combined approach provides not only accurate chemical insight on conformation, structure and molecular properties, but also benchmarking standards guiding the development of theoretical calculations. In order to illustrate these possibilities, we present the results on the conformational landscape of several carbohydrates, peptides and glycopeptides [2-4] with different biological roles. In addition, others applications of high resolution spectroscopies are showed [5-8].



- [1] E. J. Coccinero, P. Çarcabal, T. D. Vaden, J. P. Simons, B. G. Davis, *Nature* 2011, 469, 76.
- [2] I. A. Bermejo, I. Usabiaga, I. Compañón, J. Castro-López, A. Insausti, J. A. Fernández, A. Avenoza, J. H. Bustó, J. Jiménez-Barbero, J. L. Asensio, J. M. Peregrina, G. Jiménez-Osés, R. Hurtado-Guerrero, E. J. Coccinero and F. Corzana *J. Am. Chem. Soc.*, 2018, 140, 9952.
- [3] E. J. Coccinero, A. Lesarri, P. Écija, F. J. Basterretxea, J.-U. Grabow, J. A. Fernández, F. Castaño, *Angew. Chem. Int. Ed.*, 2012, 51, 3119.
- [4] E. J. Coccinero, A. Lesarri, P. Écija, Á. Cimas, B. G. Davis, F. J. Basterretxea, J. A. Fernández, F. Castaño, *J. Am. Chem. Soc.*, 2013, 135, 2845.
- [5] E. J. Juarez-Perez, L. K. Ono, I. Uriarte, E. J. Coccinero and Y. Qi, *ACS Appl. Mater. Interfaces*, 2019, 11, 12586.
- [6] M. Carini, M. P. Ruiz, I. Usabiaga, J. A. Fernández, E. J. Coccinero, M. Melle-Franco, I. Diez-Pérez and A. Mateo-Alonso *Nat. Commun.*, 2017, 8, 15195.
- [7] C. Calabrese, W. Li, G. Prampolini, L. Evangelisti, I. Uriarte, I. Cacelli, S. Melandri and E. J. Coccinero *Angew. Chem. Int. Ed.*, 2019, 131, 8525.
- [8] C. Calabrese, B. Temelso, I. Usabiaga, N. A. Seifert, F. J. Basterretxea, G. Prampolini, G. C. Shields, B. H. Pate, L. Evangelisti and E. J. Coccinero *Angew. Chem. Int. Ed.*, 2021, just accepted.

Host: Melanie Schnell / CFEL Molecular and Ultrafast Science Seminar