ELECTRIC FIELDS FOR TUNING MOLECULAR ORIENTATION IN TPD-MODIFIED GLASSES

Marta Rodríguez-López, Antonio Cappai, Claudio Melis, Luciano Colombo, Javier Rodríguez-Viejo, Marta Gonzalez-Silveira.

INTRODUCTION

ORGANIC ELECTRONIC DEVICES

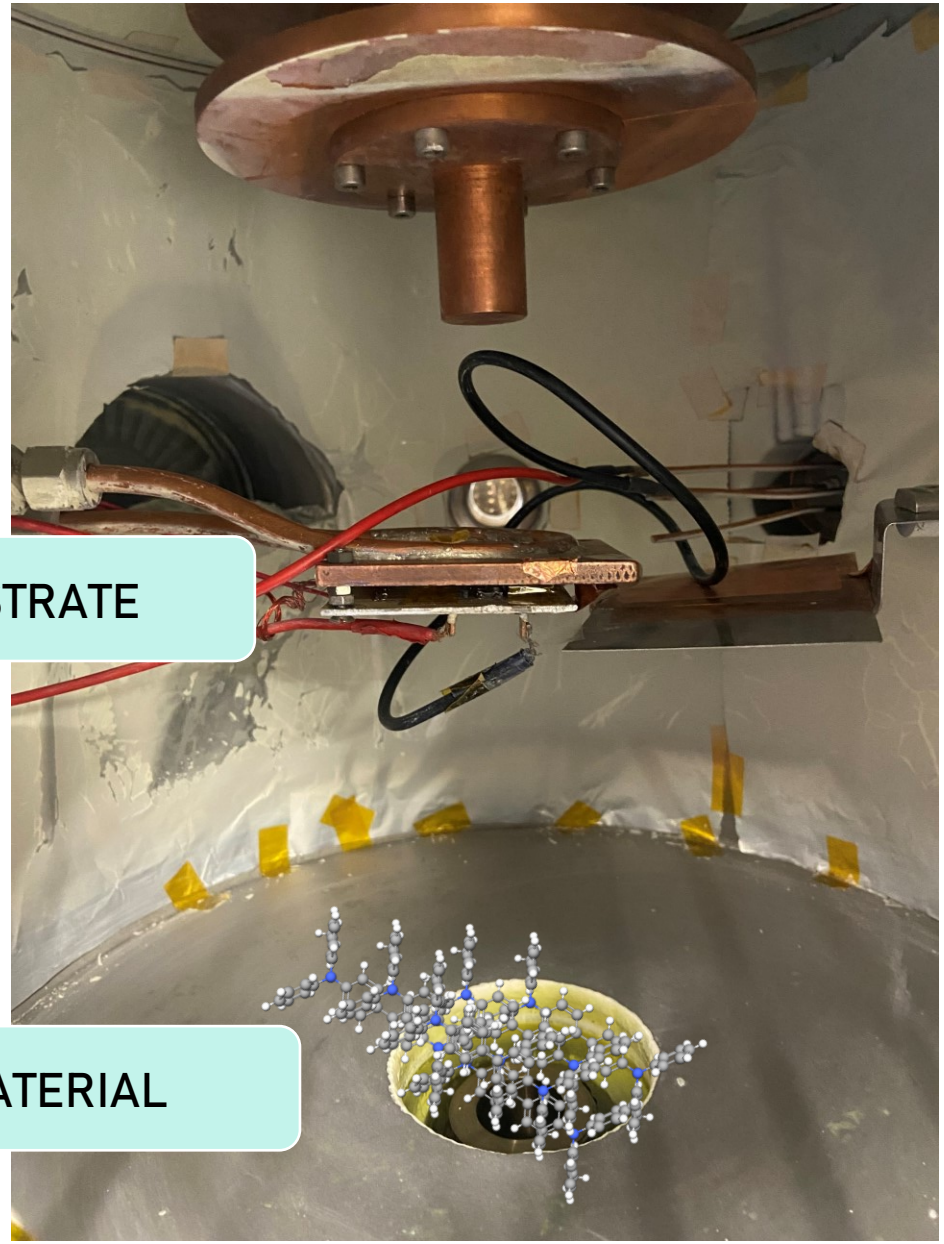
- ✓ **Glassy** organic thin films (~ 20 - 100 nm)
- ✓ Customisable
- ✗ Longevity
- ✗ Efficiency
- ✗ Low mobilities

Improved by →

- Thermal stability
- Packing
- Molecular orientation

INTRODUCTION

PHYSICAL VAPOUR DEPOSITION

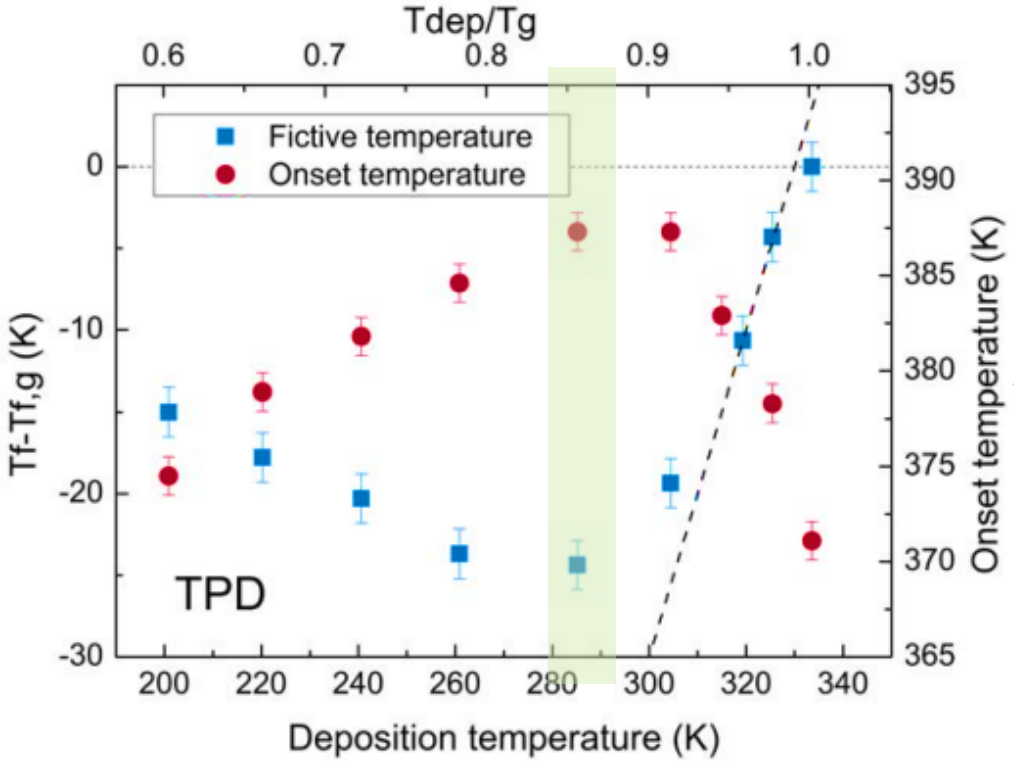


INTRODUCTION

PHYSICAL VAPOUR DEPOSITION

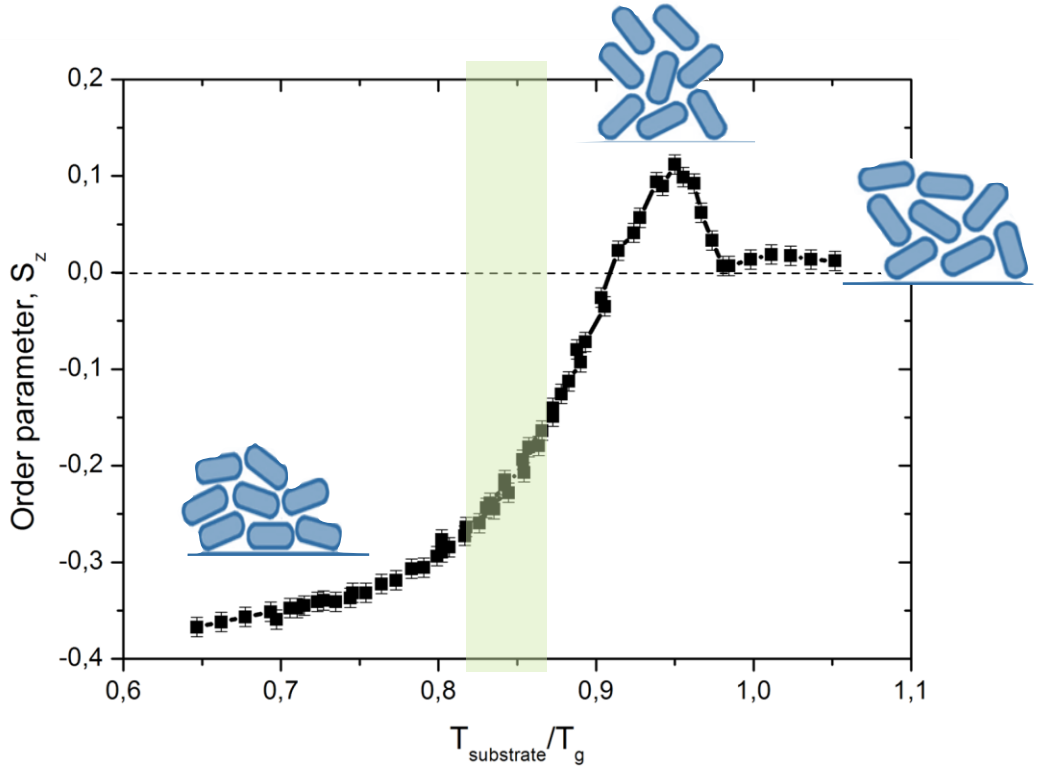
Properties controlled by substrate temperature

- Deposit ultrastable glasses



J.Ràfols-Ribé, *Organic Vapour Deposited Glasses: From Fundamental Thermal Properties to High Performance Organic Light-Emitting Diodes*, UAB (2017)

- Create a preferential orientation

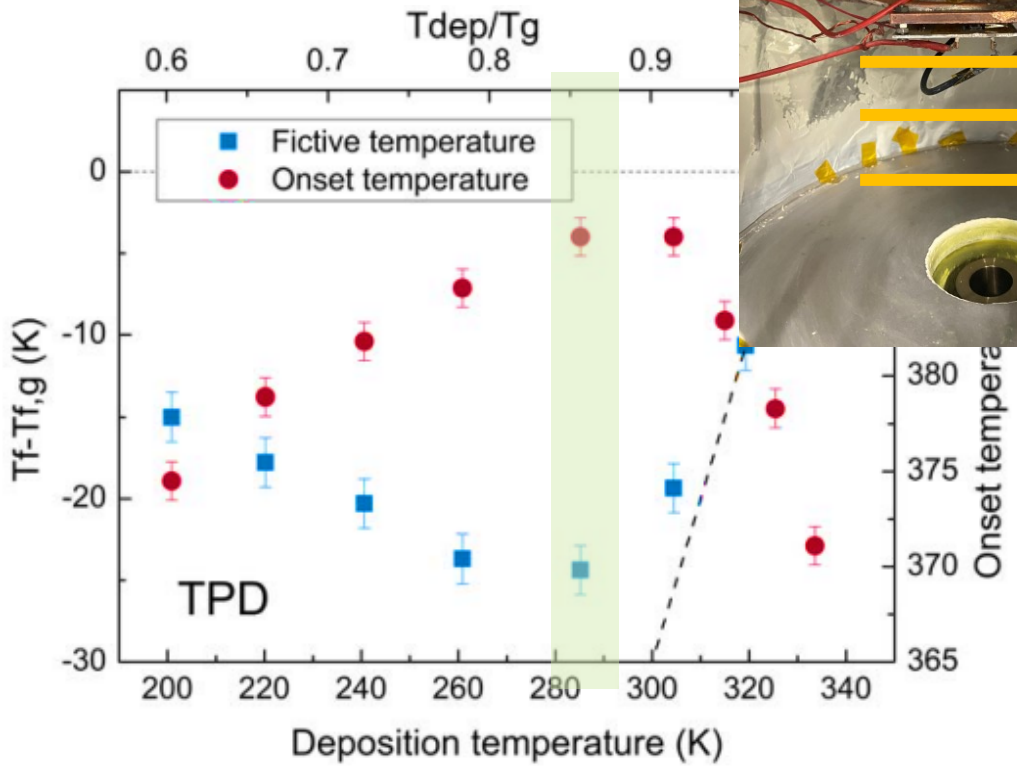


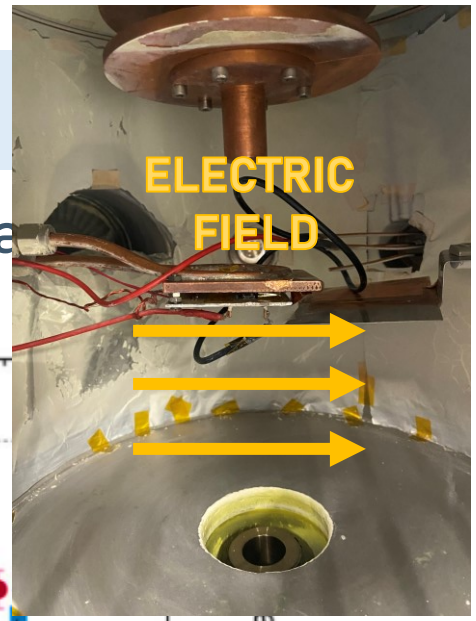
Proc. Natl. Acad. Sci. USA 112, 4227 (2015)

INTRODUCTION

OBJECTIVES

- Deposit ultrastable gla

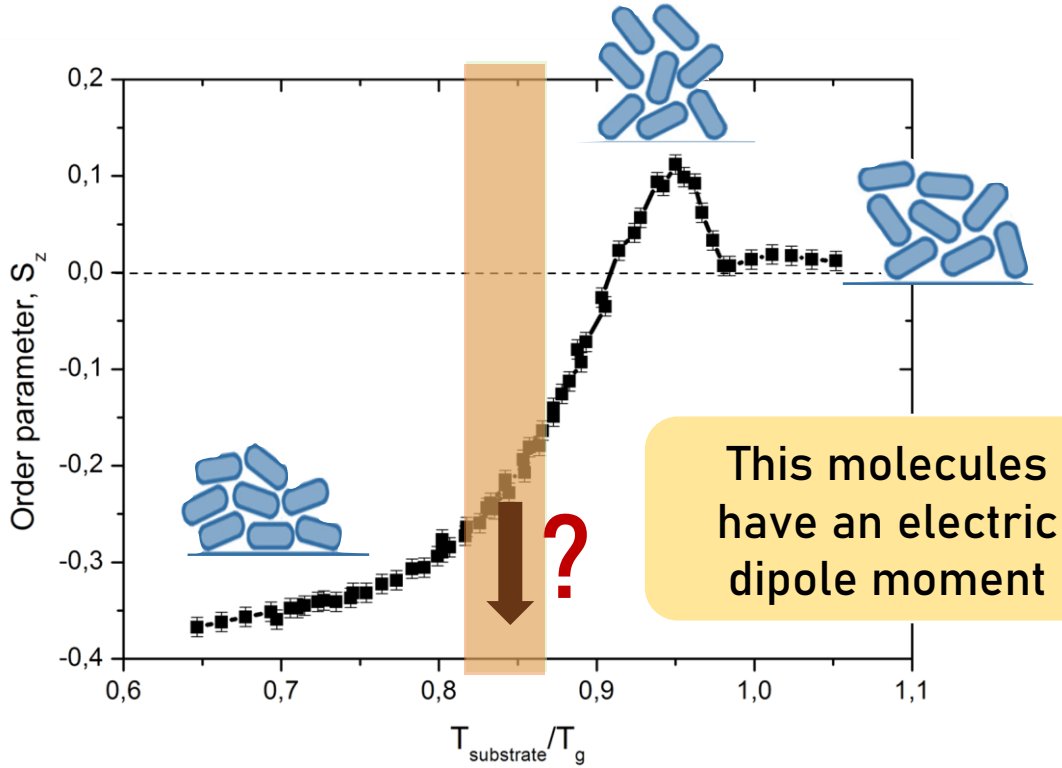




J.Ràfols-Ribé, *Organic Vapour Deposited Glasses: From Fundamental Thermal Properties to High Performance Organic Light-Emitting Diodes*, UAB (2017)

TUNE MOLECULAR ORIENTATION WITH AN ELECTRIC FIELD?

- Create a preferential orientation



This molecules have an electric dipole moment

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INTRODUCTION

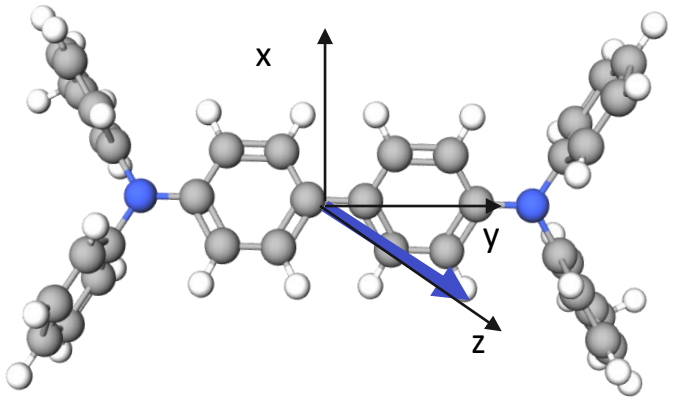
ORGANIC SEMICONDUCTINGC MOLECULES

μ DFT Calculations by Antonio Cappai
Tg experimentally determined

TPD

Tg=333 K

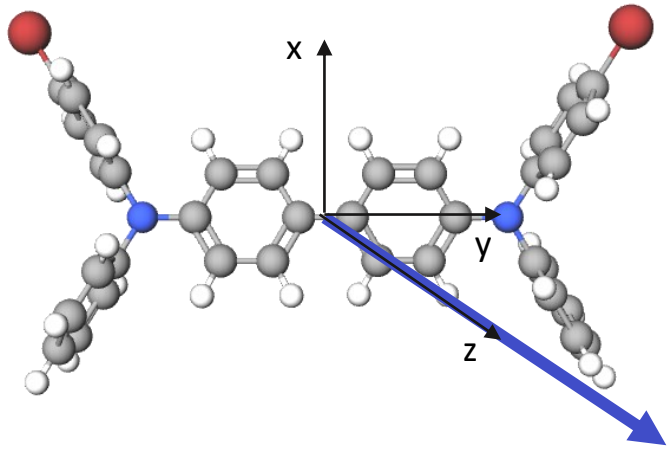
μ = 1.52 D



TPD-Br1

Tg=354 K

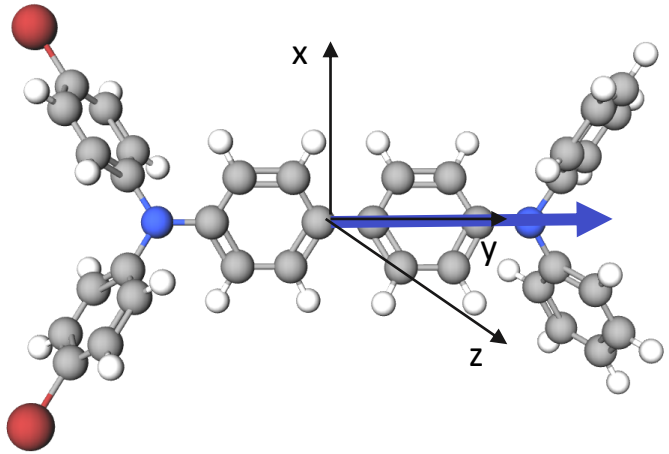
μ = 4.01 D



TPD-Br2

Tg=354 K

μ = 2.84D



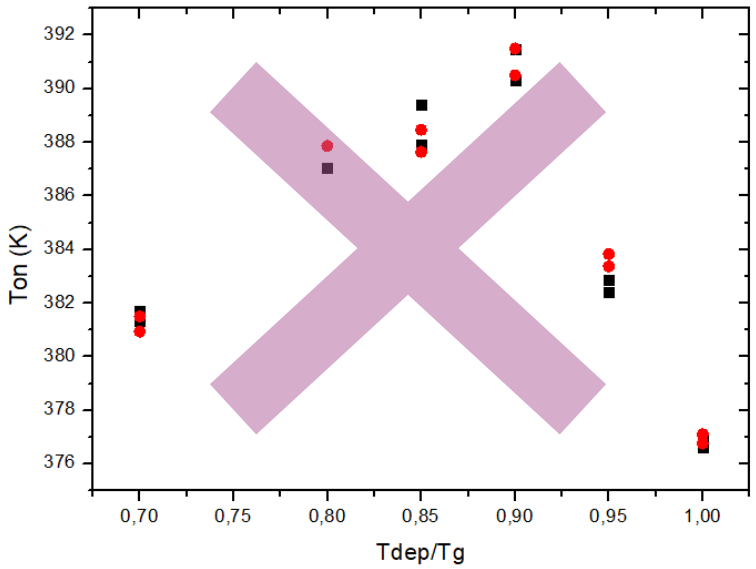
EXPERIMENTAL RESULTS

NO RESPONSE TO ELECTRIC FIELD

No electric field

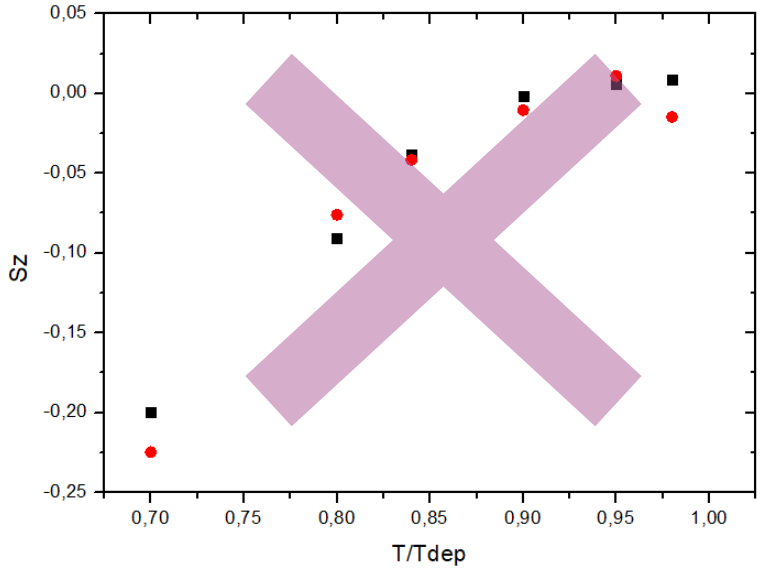
Electric field

THERMAL STABILITY



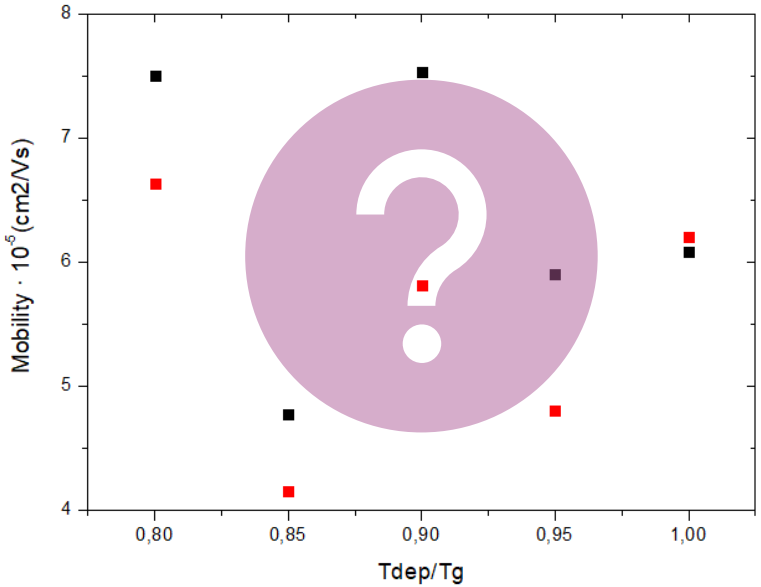
10^5 V/m

STRUCTURAL PROPERTIES



10^5 V/m

CARRIER MOBILITY



10^6 V/m

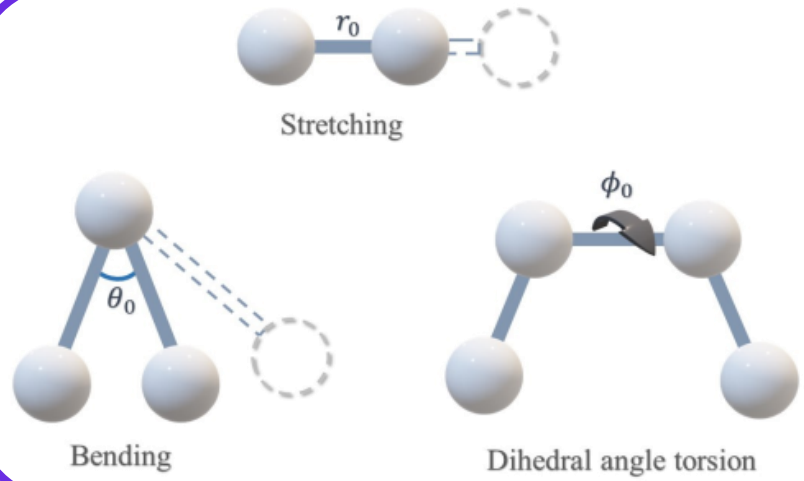
MOLECULAR DYNAMICS

SIMULATION CONDITIONS

LAMMPS software

Amber force field

DFT parameters



$$U^{bonds} = \sum_{i}^{n_b} k_i (r_i - r_0)^2$$

$$U^{angles} = \sum_{i}^{n_a} q_i (\theta_i - \theta_0)^2$$

$$U^{torsion} = \sum_{i}^{n_a} w_i (1 + \cos(n\phi_i - \phi_0)^2)$$

Bonded part

$$U^{Coulomb} = \sum_{non-bonded} \frac{q_i q_j}{r_{ij}}$$

$$U^{LJ} = \sum_{non-bonded} 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} + \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right]$$

Non-bonded part

MOLECULAR DYNAMICS

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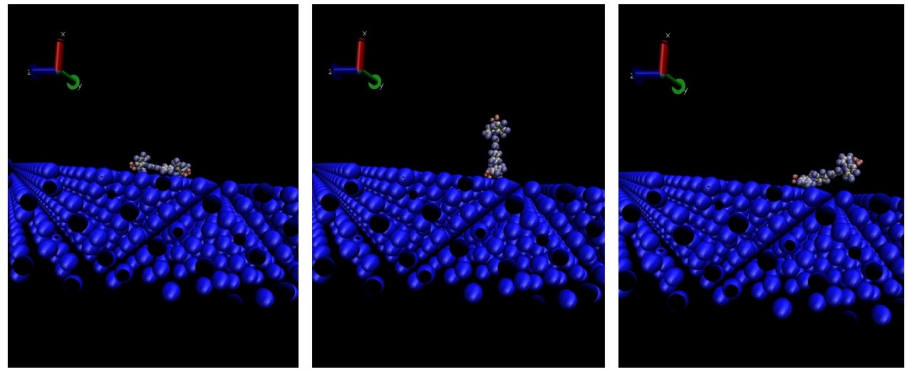
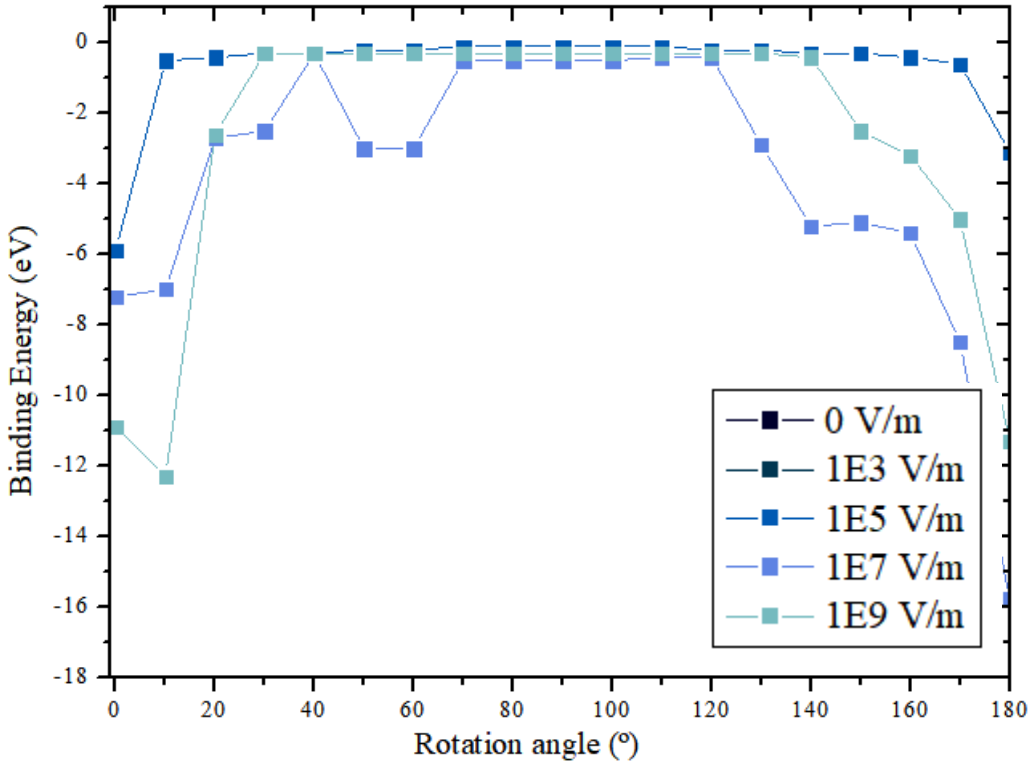
DFT parameters

Much higher electric fields!

10^9 V/m

Results for TPD-Br2





Results for TPD-Br2

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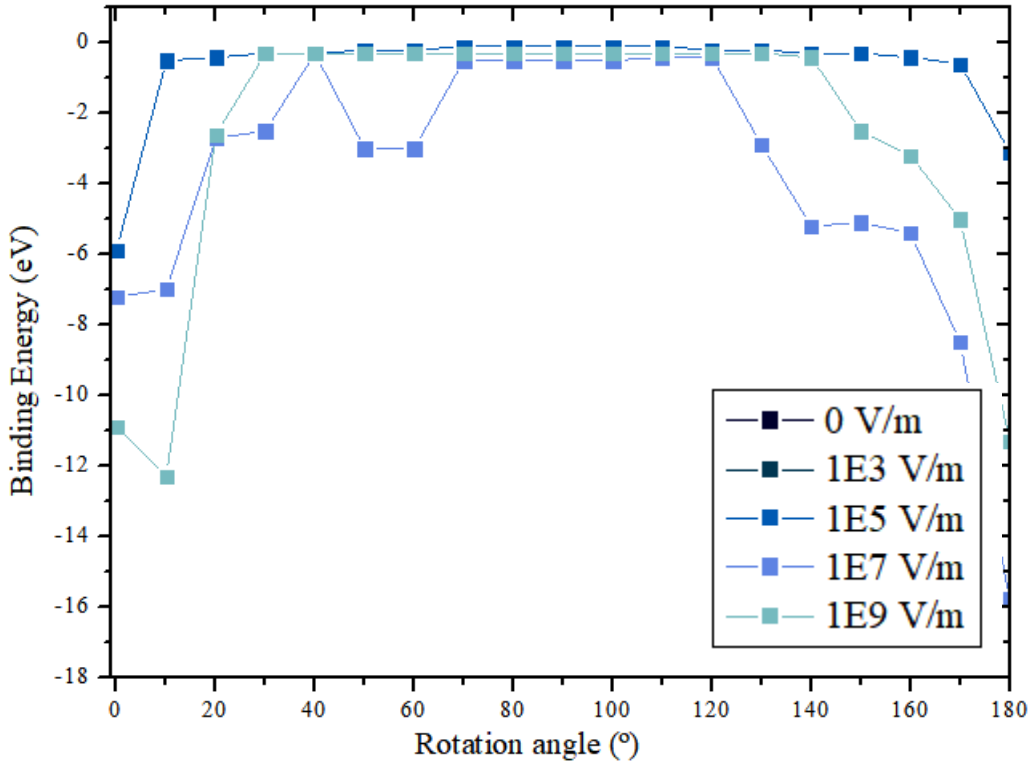


Much higher electric fields!

10^9 V/m

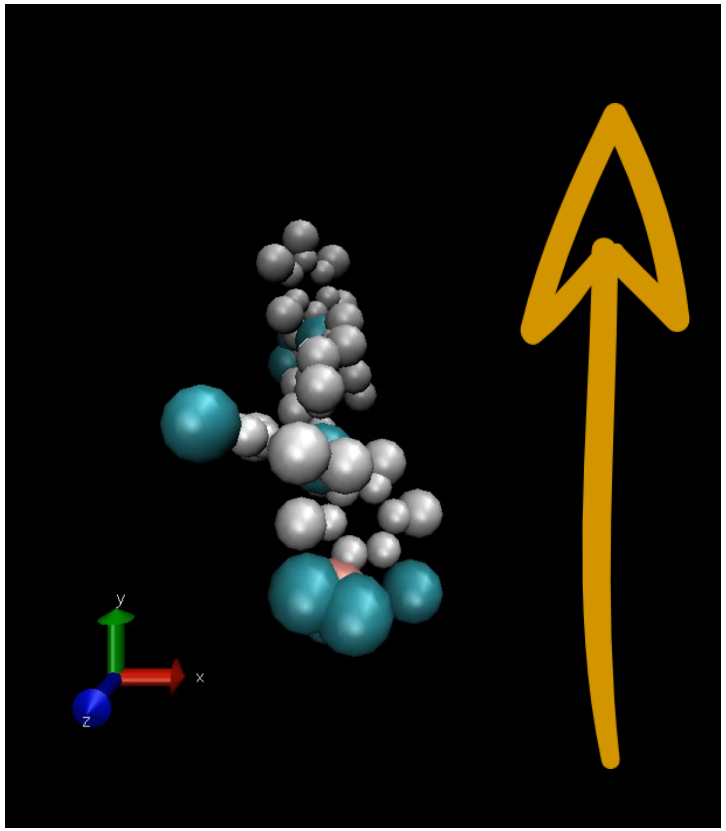
Access to the behaviour of every single molecule

Dipole moment orientation

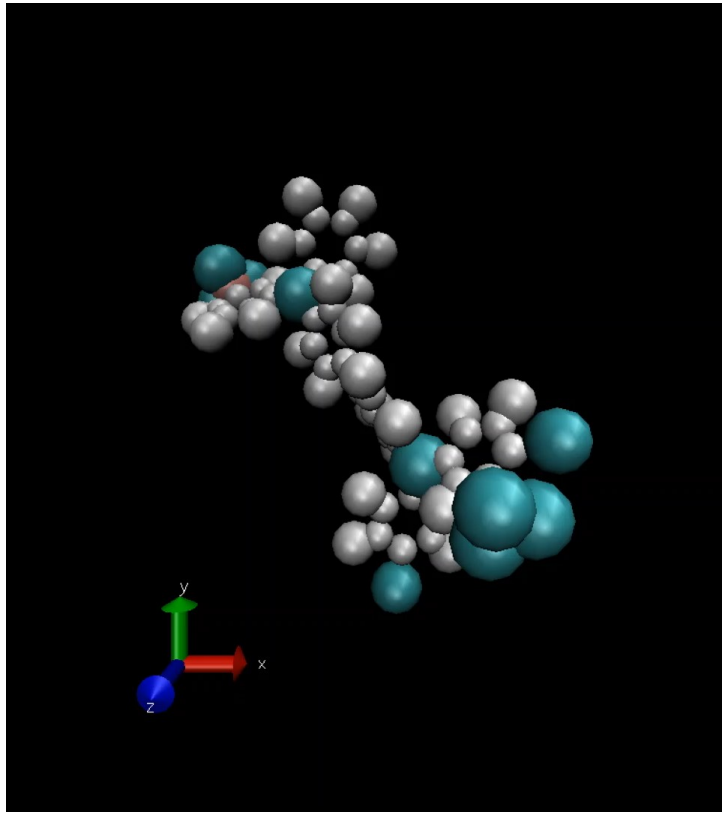
MOLECULAR DYNAMICS

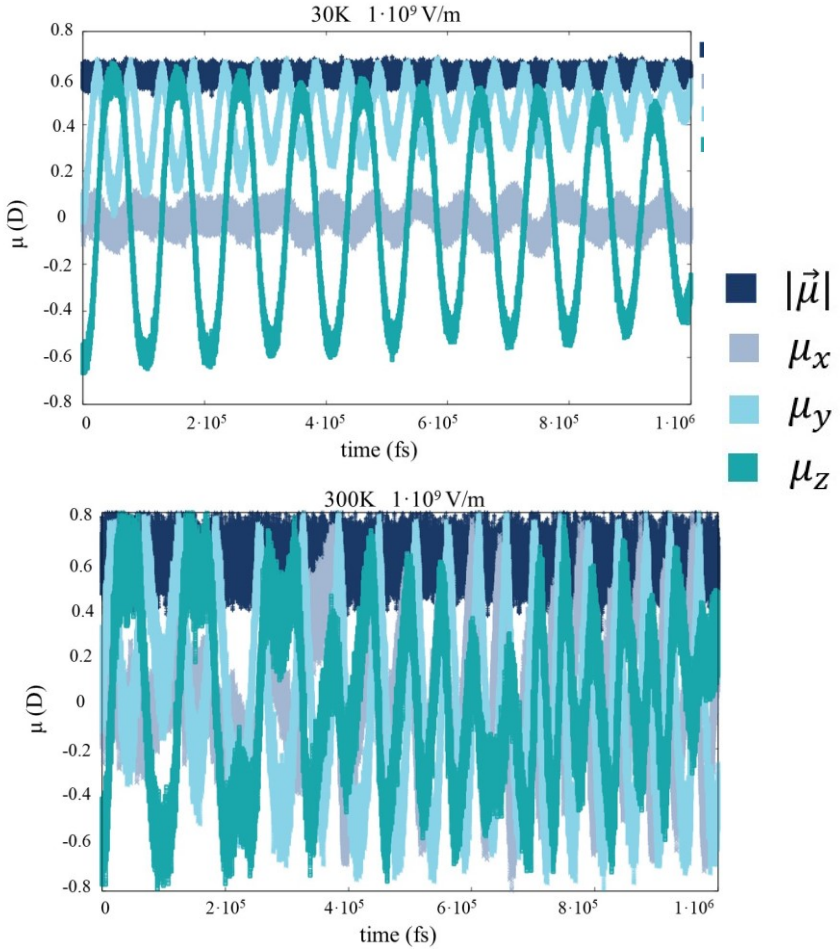
SINGLE MOLECULE – DYNAMICS

30K, 1·10⁹ V/m



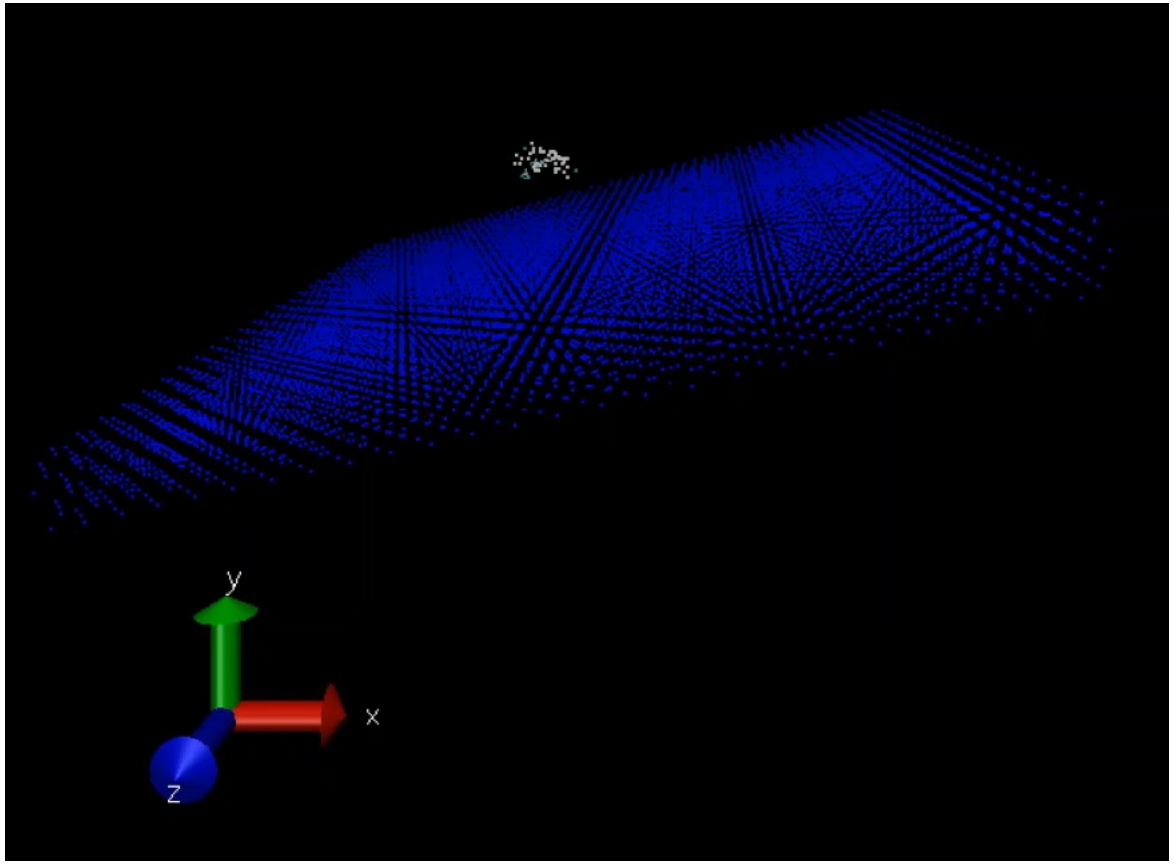
300K, 1·10⁹ V/m

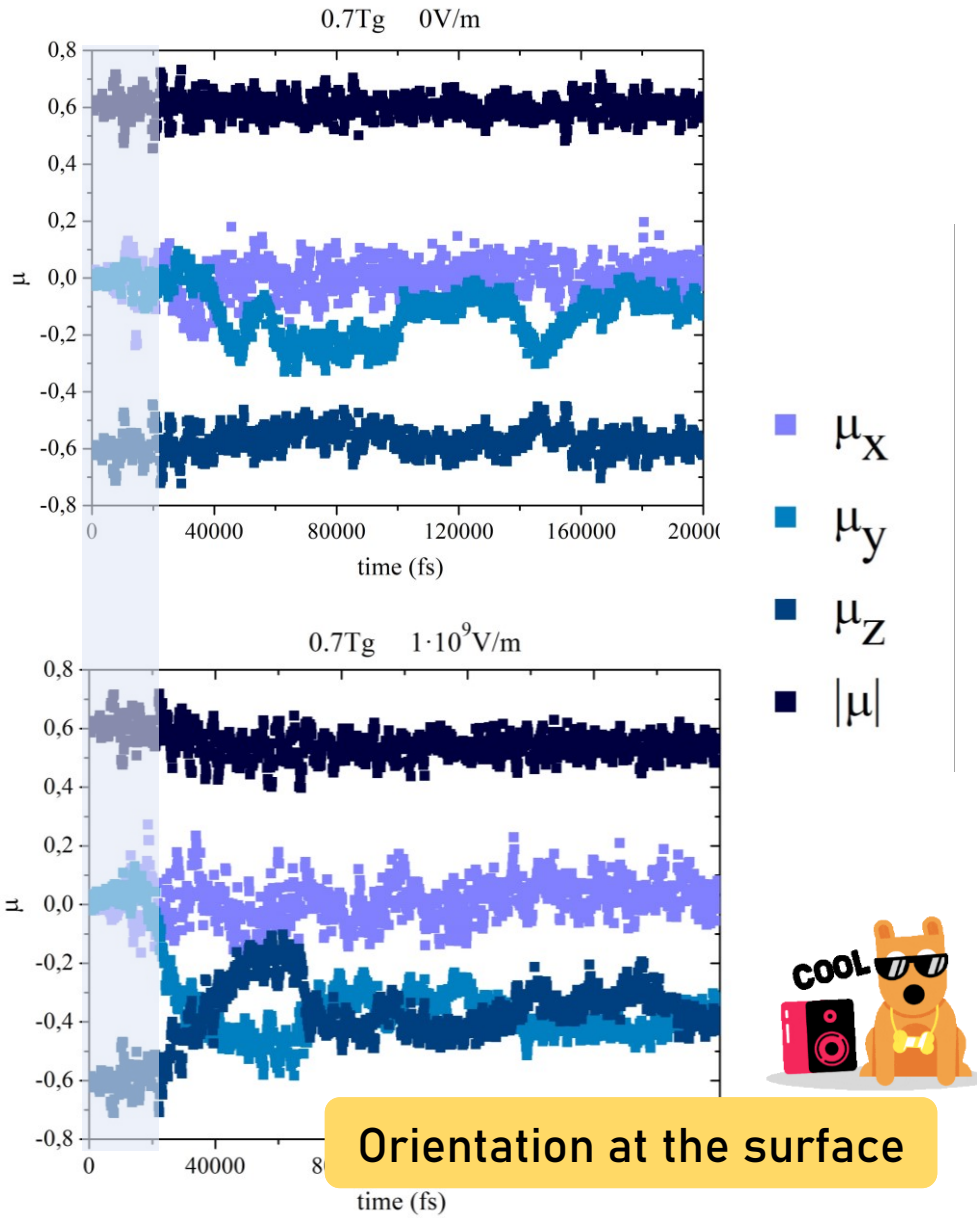




MOLECULAR DYNAMICS

SINGLE MOLECULE – DYNAMICS

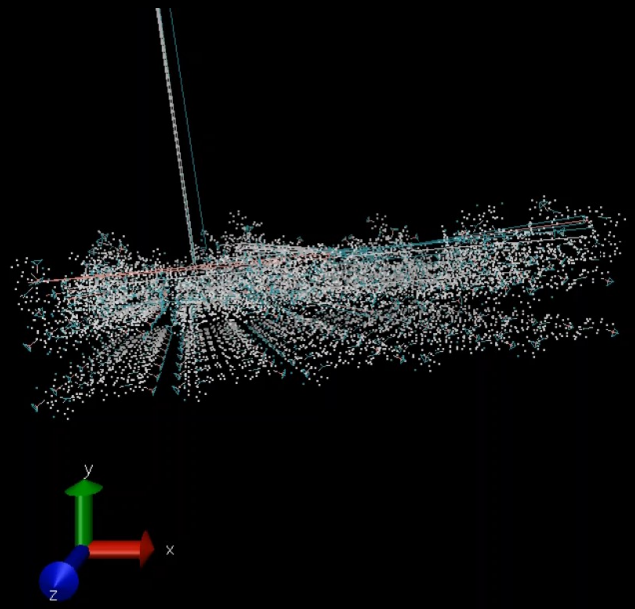


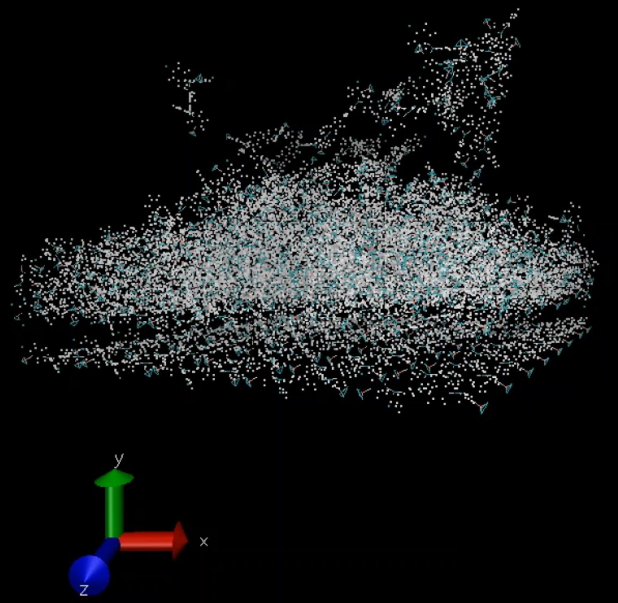


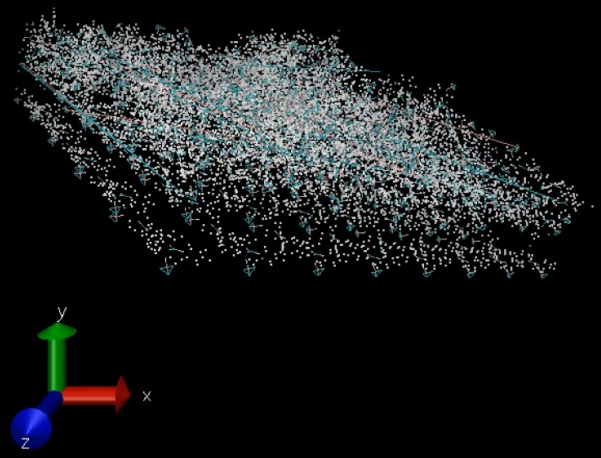
Orientation at the surface

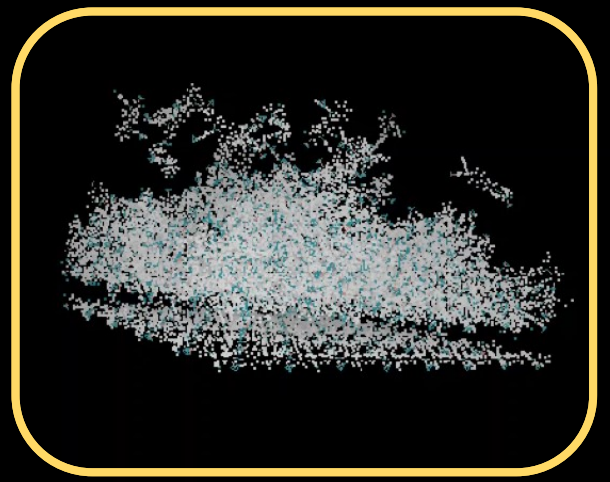
MOLECULAR DYNAMICS

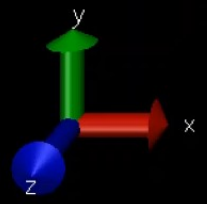
GLASS DEPOSITION





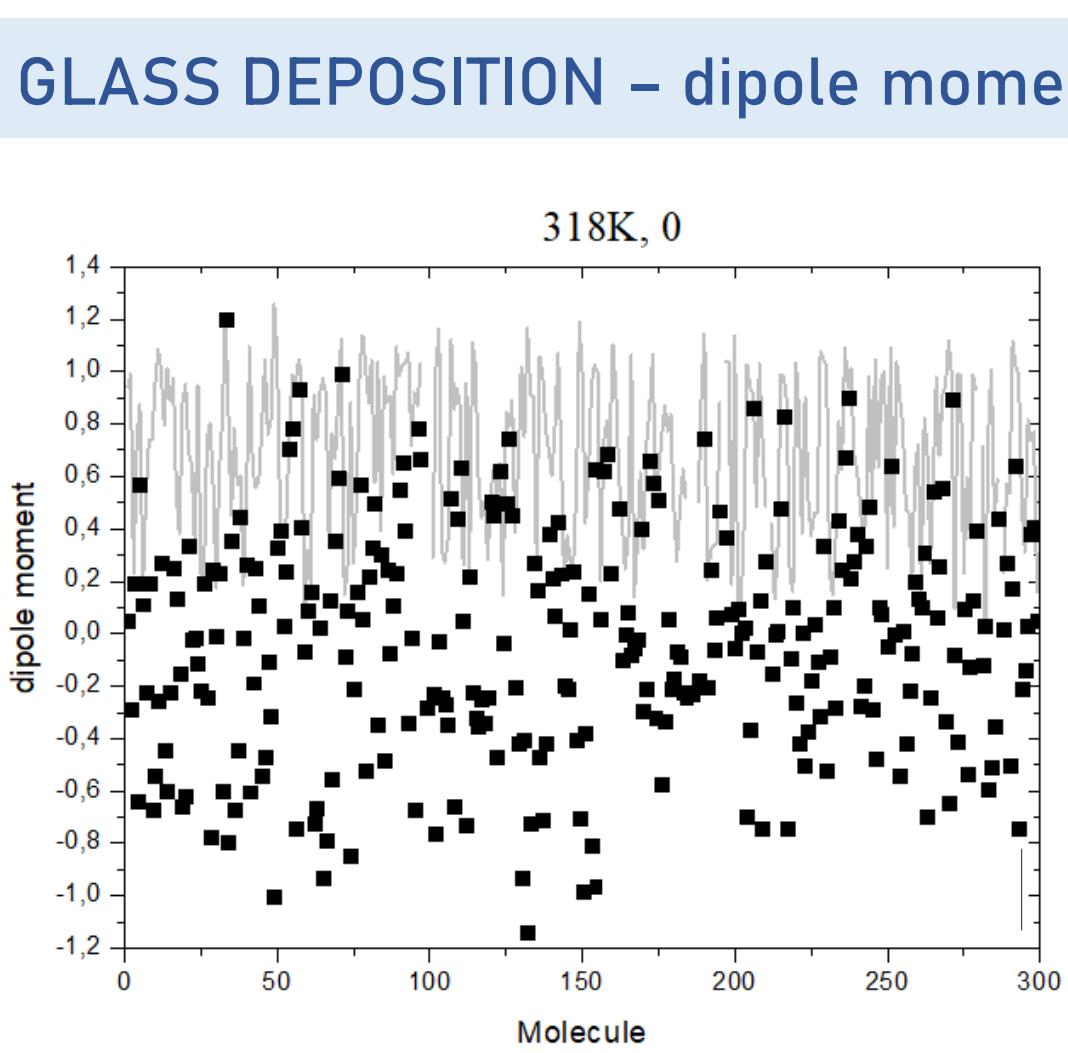


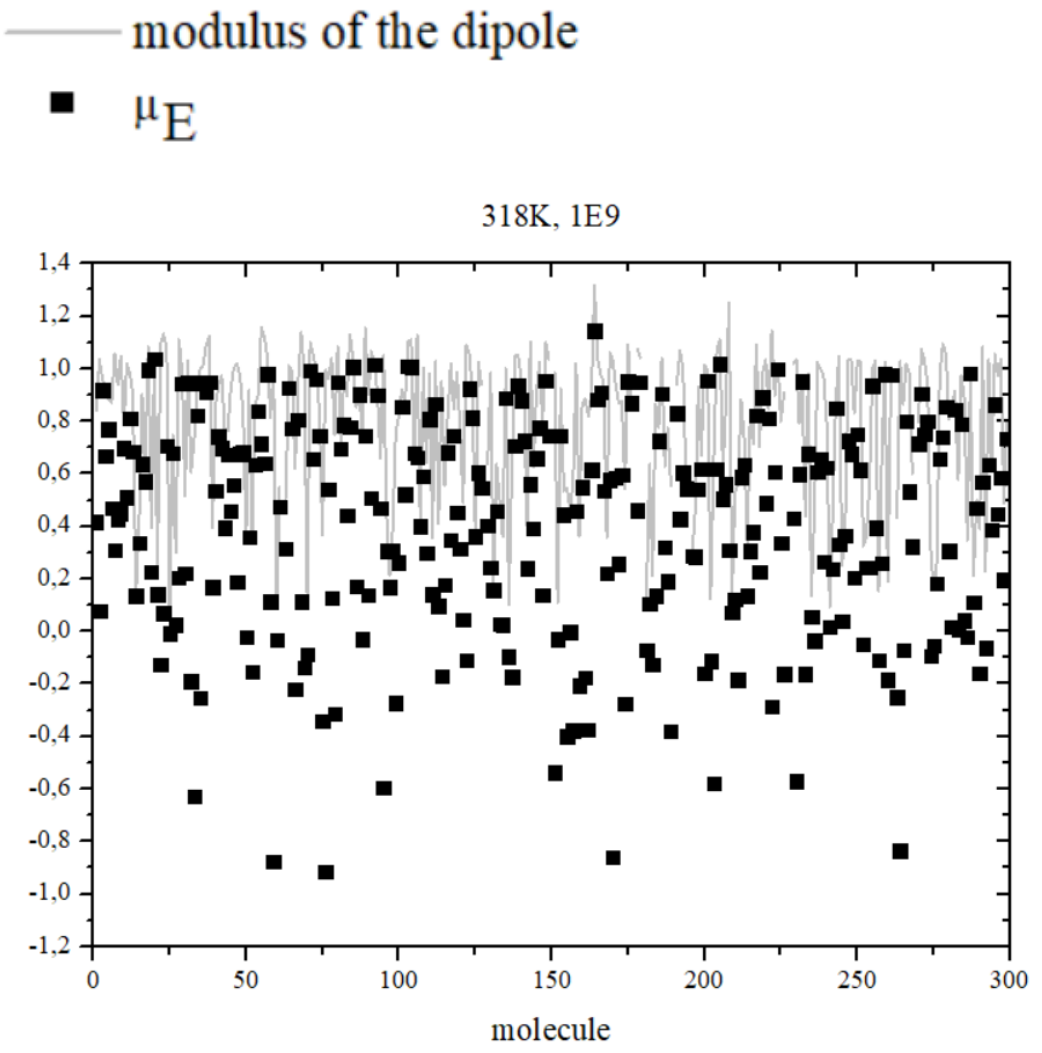




MOLECULAR DYNAMICS

GLASS DEPOSITION – dipole moment



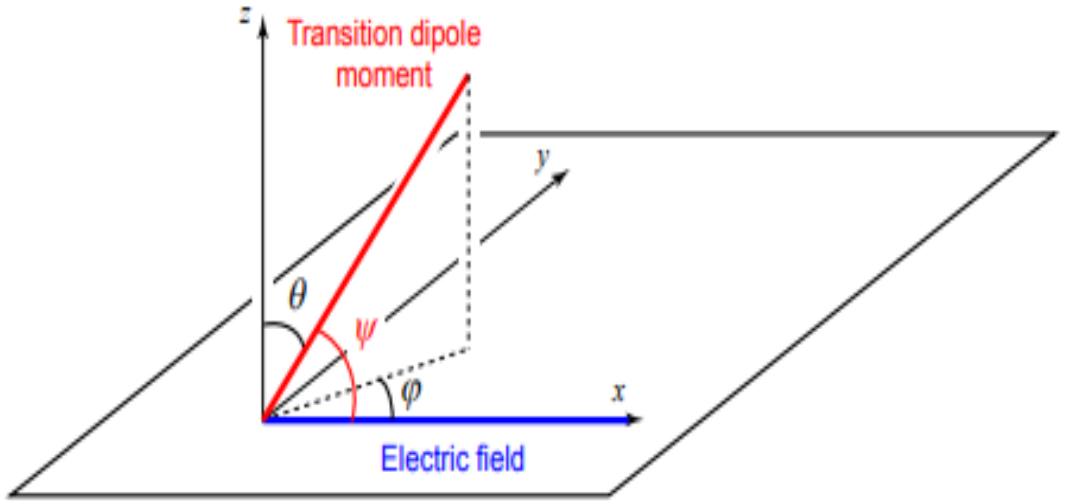


MOLECULAR DYNAMICS

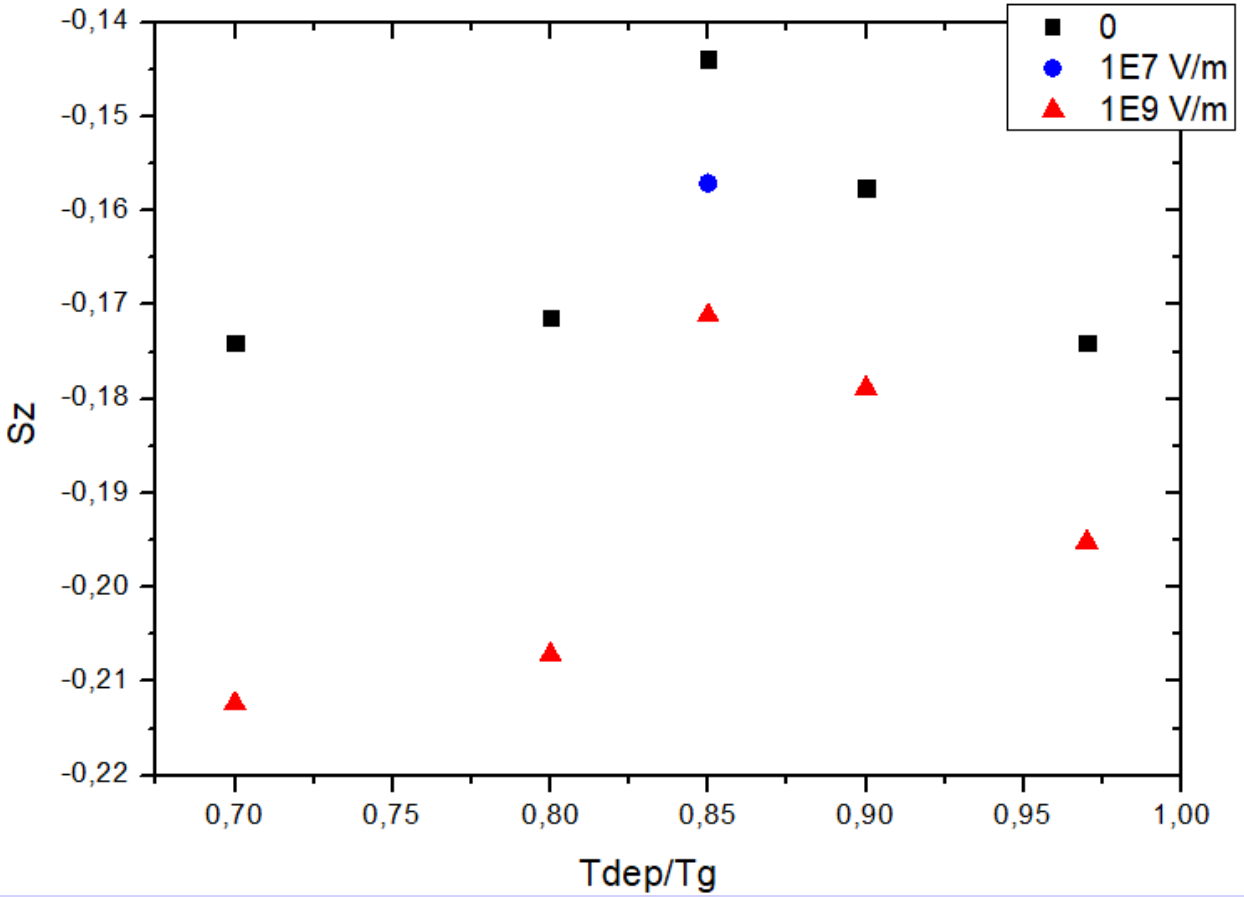
GLASS DEPOSITION - Sz

TPDs have TDM along long axis

$$S_Z = \frac{3 \cdot \langle (\cos\theta)^2 \rangle - 1}{2}$$



More horizontally oriented = Sz more negative



THANK YOU FOUR YOUR ATTENTION!

Electric fields for tuning molecular orientation in TPD-modified glasses

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Università degli Studi di Cagliari

MOLECULAR DYNAMICS

GLASS DEPOSITION

- TPD-Br substrate
- 20 x 15 molecules (28512 atoms)
- $\vec{E} = (0, 0, 10^9)$ V/m
- Thermal procedure to mimic high mobility at Surface
- ts=0,5 fs

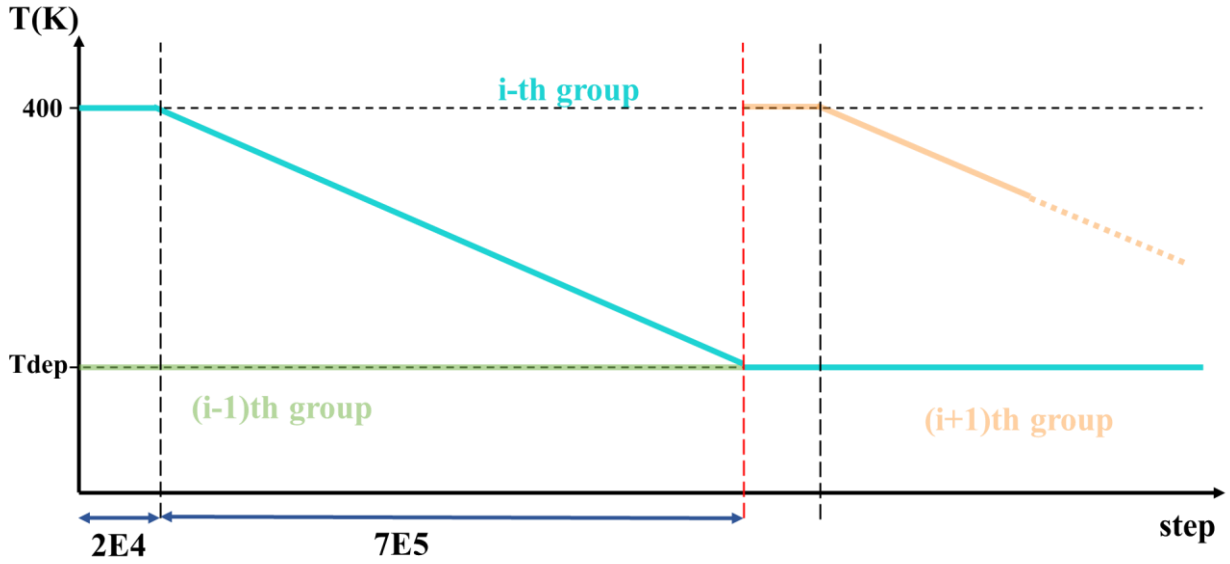

TABLE II. Gas phase Cartesian components of the electric dipole moment μ_i (in Debye) for TPD, α-NPD, TCTA and TPBi molecules before (first rows, labeled as Pristine) and after halogenation.

Pristine	$\mu_x(\pm 0.09\text{D})$	$\mu_y(\pm 0.09\text{D})$	$\mu_z(\pm 0.09\text{D})$
TPD	-0.31	0.26	0.04
α-NPD	-0.23	0.11	0.20
TCTA	-0.01	-0.01	0.00
TPBi	-4.11	-4.55	1.72
after Bromination	μ_x(D)	μ_y(D)	μ_z(D)
TPD	-0.06	4.05	0.12
α-NPD	0.90	-3.31	1.17
TCTA	-1.88	3.20	-0.06
TPBi	-1.77	5.76	1.52
after Chlorination	μ_x(D)	μ_y(D)	μ_z(D)
TPD	-0.08	3.97	0.12
α-NPD	0.93	-3.25	1.15
TCTA	-1.85	3.20	-0.04
TPBi	-1.78	5.76	1.46
after Fluorination	μ_x(D)	μ_y(D)	μ_z(D)
TPD	-0.08	2.49	0.27
α-NPD	1.05	-2.27	0.67
TCTA	-2.66	0.24	-0.02
TPBi	-0.6	5.71	1.76