# Electric fields for tuning molecular orientation in TPD-modified glasses

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## INTRODUCTION

Molecular organic glasses are nowadays gaining attention due to the great advantages they present when used in the electronics industry, such as flexibility, freedom of choice of the underlying layers, low cost, easily control of the thickness and composition and simple fabrication process. However, their lack of efficiency and long-term stability prevent their presence in our daily life. These inconveniences can be solved if those glasses are prepared by Physical Vapor Deposition (PVD) [1]. This technique permits to tune glasses properties by changing the preparation conditions such as the deposition temperature and rate. One of the key attributes that can be tuned is the spatial orientation of the molecules in the glass, differing from the random distribution that a traditional isotropic glass would have, therefore enhancing the electrical, thermal and optical properties of the glassy materials [2,3]. The orientation is mostly determined by the deposition temperature during a PVD process, which is also involved in the stability of the glass. Therefore, it is desirable to decouple these two properties – in order to obtain ultrastable glasses in which the orientation of its molecules can be chosen as demanded by the final application.

## MODEL

In this work, molecular dynamics simulations (performed by the LAMMPS package) are used for studying the electric field effect on the PVD process. Previous investigations already managed to extract properties of vapor deposited glasses, as stability and anisotropy, by building up organic molecules with Lennard-Jones model potentials [4]. Our work goes one step further, as it simulates the realistic structures of the deposited molecules using the GAFF force field. External electric field is applied to the system in order to determine if it is possible to change the orientation imposed by the substrate temperature.

## DESCRIPTION

We are studying how molecules in a simulated vapor deposited glass behave under the application of an external electric field of up to $10^9$ V/m. The goal is to change the imposed orientation by the deposition temperature. To do so, the molecules used for this work are a modified version of the commercially available TPD, TPD-Br. This later molecule has a larger dipole moment while maintaining the shape and the semiconductor behavior. In this context, different situations have been investigated to extract when and under which conditions there is an effect of the field to the orientation of the dipole moment, including static and dynamic depositions of single and multiple molecules. Useful parameters obtained in the laboratory, such as the order parameter, can be extracted from the simulations too.

## CONCLUSION

The work concludes that the effect of the electric field is produced at the top of the surface, where the degrees of freedom are reduced, taking advantage of the surface diffusion. These

simulations are a complement of an experimental work that intends to affect the orientation of the molecules in real systems. Therefore, the parameters obtained in the calculations can be compared to the ones obtained in the laboratory.

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