Multi-Scale Molecular Simulation of Liquid Crystal Mesogens: From Atomistic to Efficient Coarse-Grained Models

A. Díaz-Acosta[1*], I. Adroher-Benítez[1], A. Patti[1,2,3]
[1]Department of Applied Physics, University of Granada, Granada, Spain
[2]Department of Chemical Engineering, University of Manchester, UK
[3]Carlos I Institute of Theoretical and Computational Physics, Granada, Spain
*adacosta@ugr.es

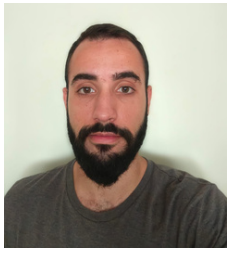
Liquid crystals represent fascinating states of matter that blend properties of both isotropic fluids and crystalline solids. They come in different phases according to the structure of their constituents and the resulting positional and orientational ordering. Nematic (N) phases emerge when alignment dominates, while smectic (Sm) phases are layered structures exhibiting both orientational and positional ordering. This work presents a comprehensive multi-scale computational investigation of a family of board-shaped mesogens, recently characterized experimentally by Lehmann's group [1], with a particular focus on their potential for self-assembling into liquid crystal phases.

Through atomistic Molecular Dynamics simulations, in our first work [2] we have systematically characterized the structural and dynamic properties of these systems. Our analysis reveals that two mesogens exhibit dominant orientation along their main axis, forming a nematic and smectic-A phase, respectively. Dynamic analysis unveils heterogeneous molecular motion and preferential intra-layer diffusion in smectic-A phase revealed by van Hove self-correlation functions. Building upon these atomistic insights, we address the fundamental challenge of computational complexity in molecular simulations by developing efficient coarse-grained (CG) models. Our systematic bottom-up approach employs force matching methodology [3] to derive effective potentials that preserve essential physicochemical properties while dramatically reducing computational cost. The CG model construction involves strategic atomic grouping into representative beads and parametrization using the Bottom-up Open-source Coarse-graining Software (BOCS) [4], enabling simulations of larger systems over extended timescales.

This multi-scale methodology bridges the gap between detailed molecular understanding and practical computational efficiency, providing both fundamental insights into liquid crystal phase behavior and a powerful framework for studying complex mesogenic systems.

References

[1] M. Lehmann, S. Maisch, N. Scheuring, J. Carvalho, C. Cruz, P. J. Sebasti~ao and R. Y. Dong. From molecular biaxiality of real board-shaped mesogens to phase biaxiality? On the hunt for the holy grail of liquid crystal science, *Soft Matter*, **15**, 8496 (2019).
[2] A. Díaz-Acosta, I. Adroher-Benítez, I. Zerón, A. Patti. Atomistic insights into liquid crystals of board-like molecules via molecular dynamics simulation, *JCP*, **161**, 234902, (2024).
[3] F. Ercolessi and J. B. Adams. Interatomic Potentials from First-Principles Calculations: The Force-Matching Method, *EPL* **26** 583 (1994).
[4] Nicholas J. H. Dunn, Kathryn M. Lebold, Michael R. DeLyser, Joseph F. Rudzinski, and W.G. Noid, BOCS: Bottom-up Open-source Coarse-graining Software, *JCPB*, **122**, 3363-3377, (2018)



Adrián Díaz Acosta studied Chemistry at the University of Huelva, where he also completed a Master's degree in Molecular Simulation jointly offered with the International University of Andalusia, graduating with the highest academic distinction from the University of Huelva. He is currently a PhD candidate in the Department of Applied Physics at the University of Granada, under the supervision of Prof. Alessandro Patti.

His research interests lie in the atomistic and coarse-grained modelling of molecular liquid crystals, aiming to predict their structural organization, dynamic behavior, and potential technological applications.