Molecular Dynamics Simulations of Small Organic Molecules in Confined Spaces

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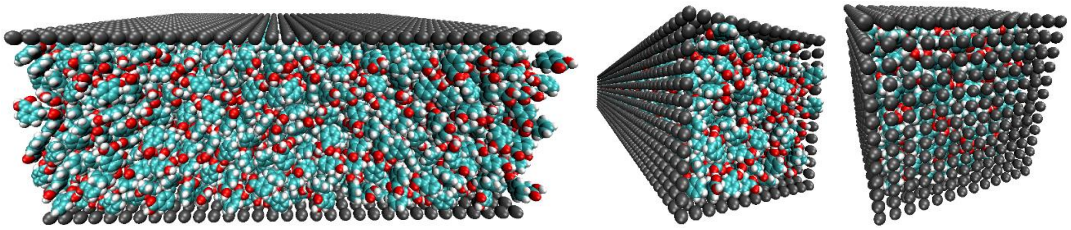
Nucleation is the main kinetic step in the formation of any crystal lattice. Despite advances in experimental techniques and computational methods [1,2], the atomic-level mechanism of nucleation is still not understood. We tackle the problem by means of classical Molecular Dynamics simulations, with the goal of exploring the early stages of the nucleation event, which are not easily amenable to experimental investigations. We are currently developing Milano Chemistry Molecular Simulation (MiCMoS) [3,4], a multi-purpose software for condensed-phase studies of small organic molecules in both static and dynamics flavors. The software is currently released under a Creative Commons license and can be downloaded free of charge for Academic users [5].



We here present a new module of MiCMoS able to carry out molecular dynamics simulations in confined systems. It is known that confinement can effectively restrict the phase space of the interacting units, fostering aggregation phenomena that may lead to (partially) ordered patterns [6]. Using simple and computationally cheap van der Waals barriers, we model three different classes of confined systems, namely a nanolayer, a nanotube and a nanocavity, having wall distances of ~ 40 Å. The new algorithm is applied to benzoic acid, a very simple rigid test case. We show that the behavior of the liquid in confined spaces differs from the bulk one, due to both the limited volume and the reduced dimensions of the accessible regions of the phase space. The comparison with free liquids and nanodroplets allows to gain insights into the impact of confinement on the formation of molecular aggregates in small organic molecules. Our findings will contribute to the understanding of the mechanism of nucleation and its relationship with confinement.

References

[1] Urquidi O et al. In Situ Optical Spectroscopy of Crystallization: One Crystal Nucleation at a Time. Proc. Natl. Acad. Sci. 2022;119(16):e2122990119.
[2] Nakamuro T et al. Capturing the Moment of Emergence of Crystal Nucleus from Disorder. J. Am. Chem. Soc. 2021;143(4);1763–1767.
[3] Gavezzotti A, Lo Presti L and Rizzato S. Molecular Dynamics Simulation of Organic Materials: Structure, Potentials and the MiCMoS Computer Platform. CrystEngComm 2022;24(5);922–930.
[4] Gavezzotti A, Lo Presti L and Rizzato S. Mining the Cambridge Database for Theoretical Chemistry. Mi-LJC: A New Set of Lennard-Jones-Coulomb Atom-Atom Potentials for the Computer Simulation of Organic Condensed Matter. CrystEngComm 2020;22(43):7350–7360.
[5] Lo Presti L, Gavezzotti A. MiCMoS (MIlano Chemistry MOlecular Simulation) 2.1; Università degli Studi di Milano: Milano, 2022; https://sites.unimi.it/xtal_chem_group/index.php
[6] Cámara L and Bresme F. Molecular dynamics simulations of crystallization under confinement at triple point conditions. J. Chem. Phys. 2003;119;2792