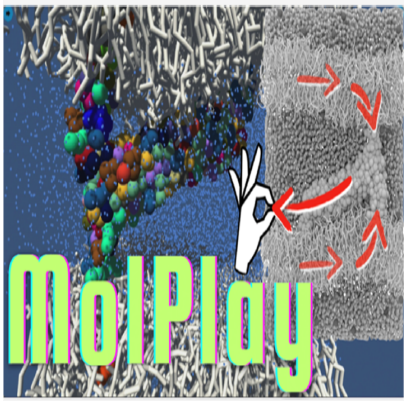
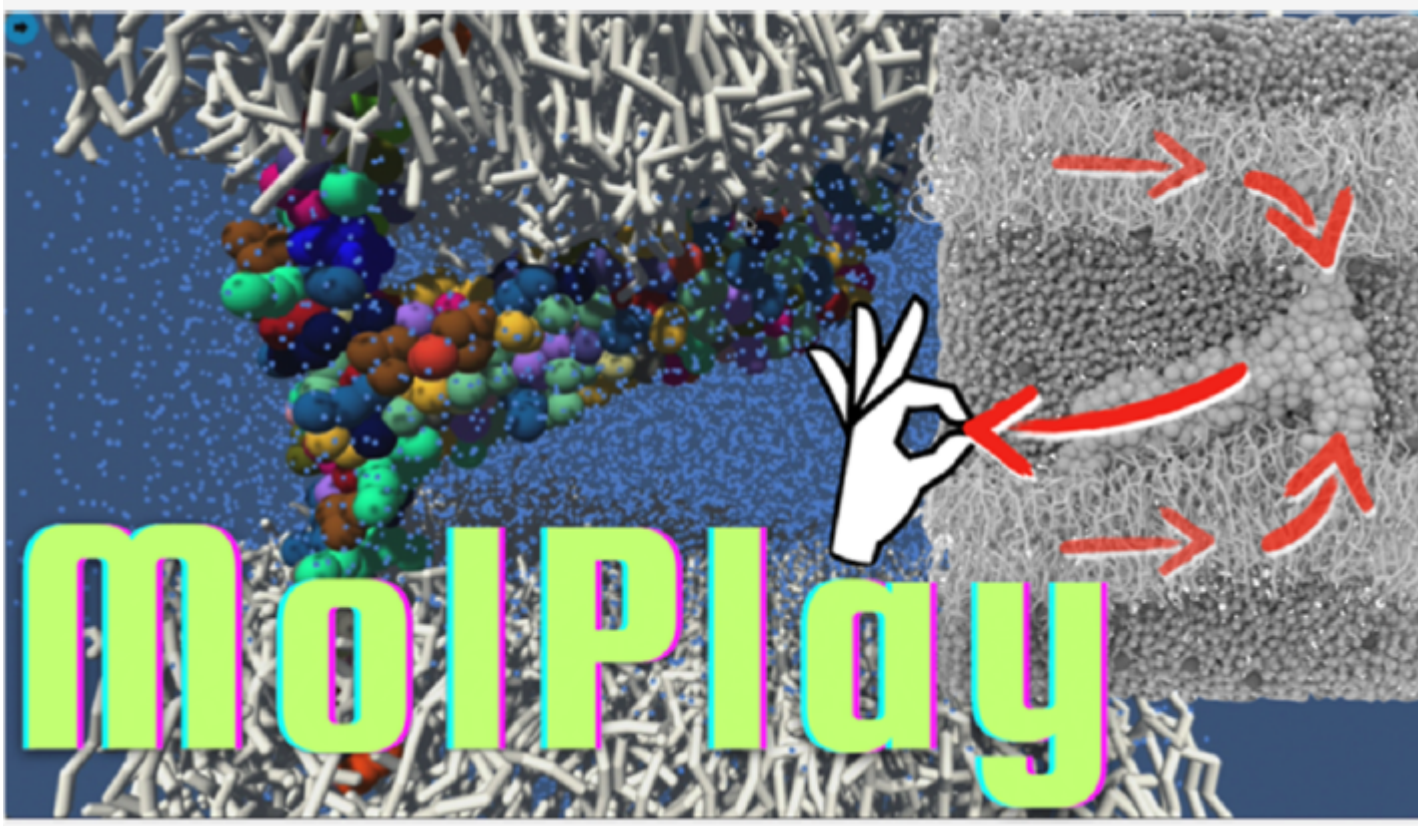


MolPlay: Democratizing Interactive Molecular Simulations and Analyses with a Portable, Turnkey Platform

Description

M. Baaden, *J. Phys. Chem. B* 2024 https://doi.org/10.1021/acs.jpcb.4c04712

Computer-based tools for visualizing and manipulating molecular structures in real-time hold immense potential for accelerating research and improving education, but are only used to a limited extent. This paper explores the possibilities of these powerful techniques. It presents a classification of common interactive modeling tasks, such as assembly, deformation, sampling of rare events, and relevant use cases, especially for studying membranes and membrane proteins. The MolPlay platform provides a ready-to-use software environment with a curated set of hands-on examples to democratize access to Interactive Molecular Simulations and Analyses (IMSA).



These research tools allow researchers to visualize, manipulate, and study digital models of molecules in real-time and can be started directly from a small, portable storage device. The portable, self-contained nature of MolPlay enables versatile deployment scenarios ranging from outreach to teaching in computer laboratories to facilitating the distribution of research software. Initial tests at an international workshop have shown that MolPlay appeals to different target groups and lowers the access barriers to IMSA. By consolidating more than a decade of expertise into one accessible platform, MolPlay represents a significant step toward the broader adoption of these underutilized but powerful computational techniques in education and research.

The MolPlay website, https://molplay.mol3d.tech, provides all relevant complementary information. This includes instructions and ISO images (single files containing all the data of a CD, DVD, or other storage device) for deploying MolPlay through a bootable USB stick.