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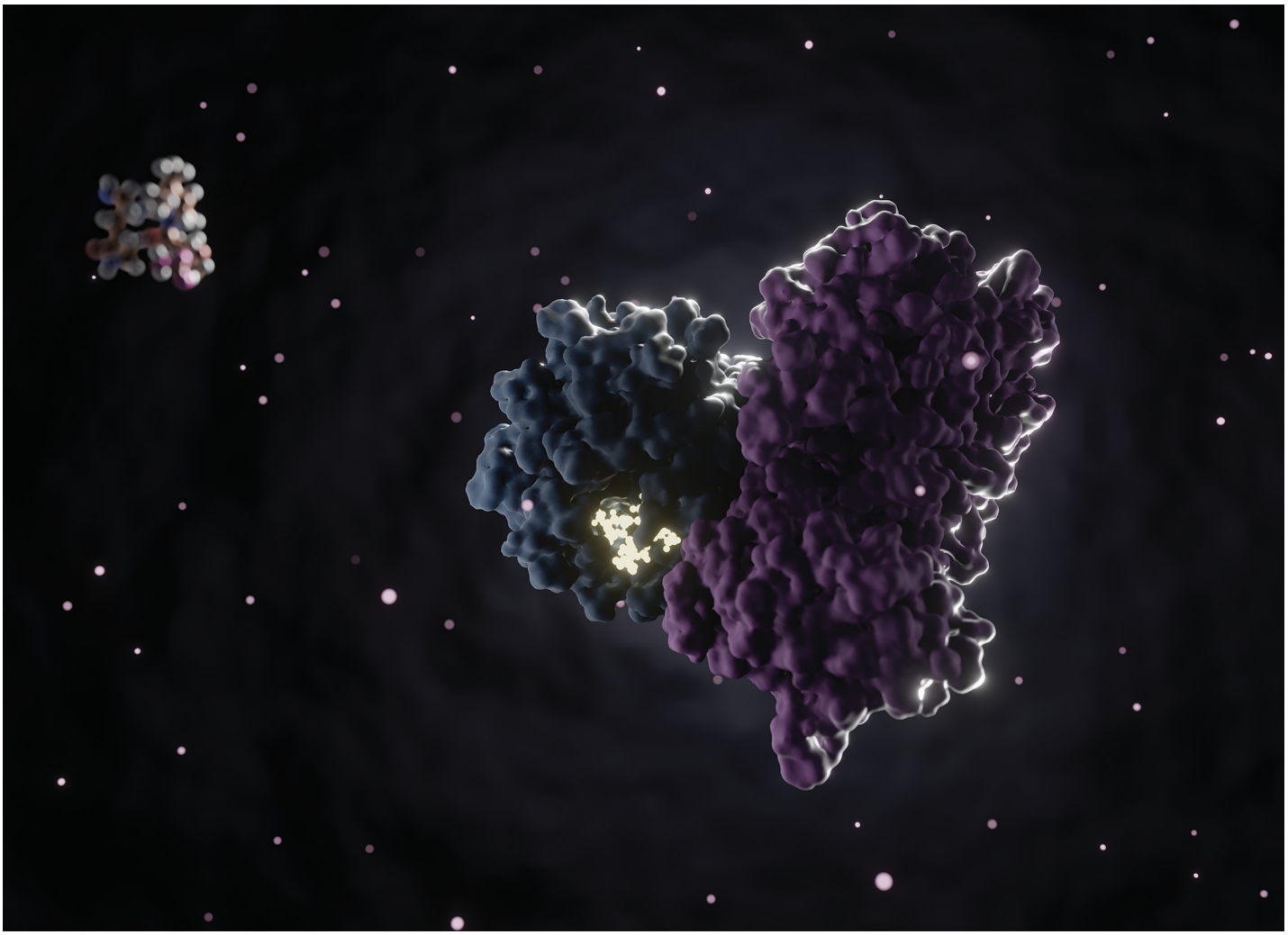

Showcasing research from the computational mechanobiology group of Dr Zhenhai Li at Shanghai University, China and the group of Prof. Dechang Li at Zhejiang University, China.

Binding kinetics study of SARS-CoV-2 main protease and potential inhibitors *via* molecular dynamics simulations.

With REMD simulation, we successfully estimated the binding kinetics of four inhibitors to the M^{pro} of SARS-CoV-2. The newly designed inhibitor PF-07321332 exhibited the highest binding affinity and specificity to the catalytically activated site of M^{pro} by forming multiple hydrogen bonds. The image shows a PF-07321332 molecule inserted into the catalytic site, which blocks the enzymatic activity and potentially stops the replication of the virus.

Image reproduced by permission of Dr Zhenhai Li.

As featured in:

See Dechang Li, Zhenhai Li *et al.*, *Phys. Chem. Chem. Phys.*, 2023, **25**, 15135.

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