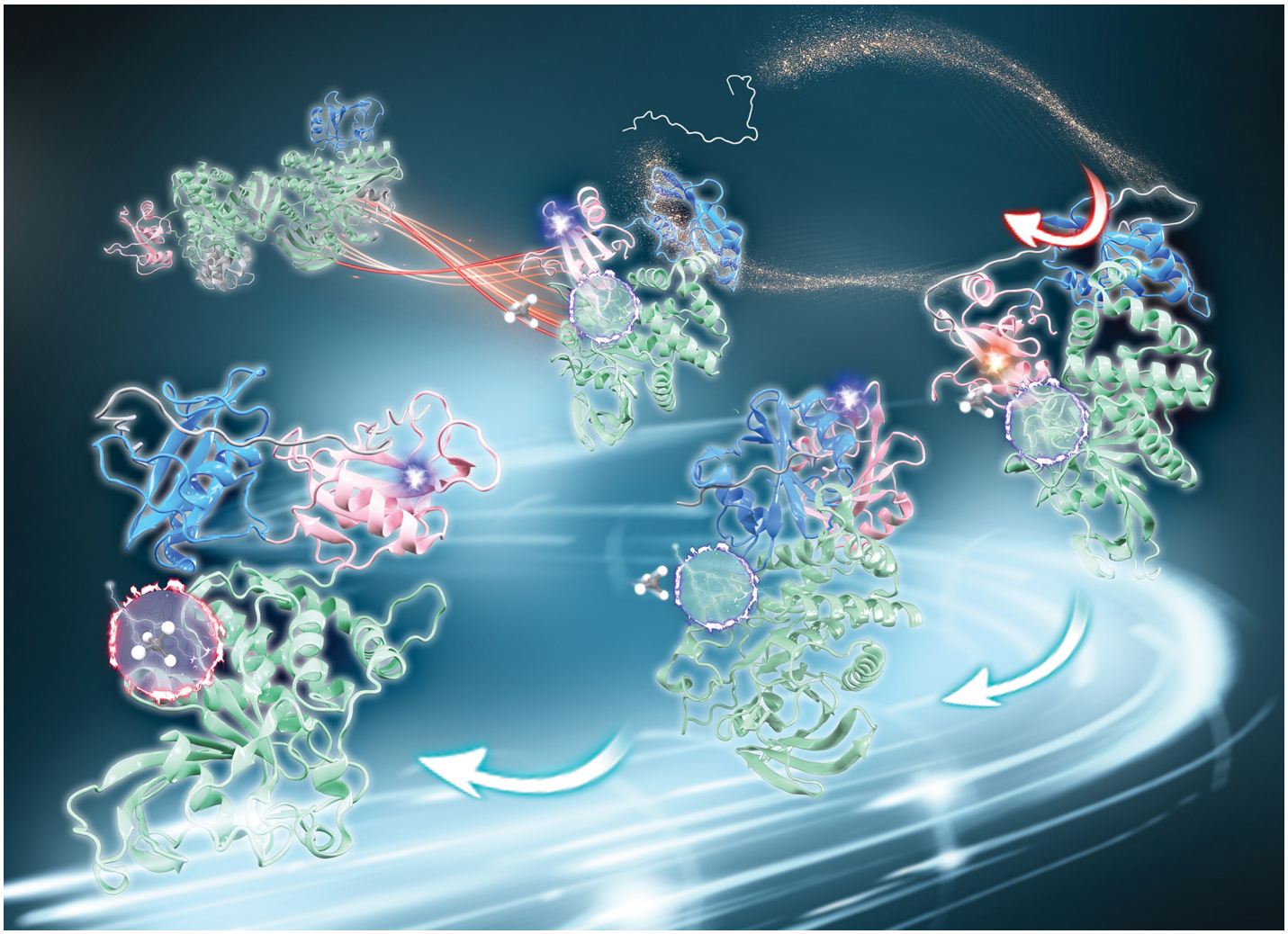

Showcasing research from the group of Professor Luo Ting at Sichuan University and Professor Hu Jianping at Chengdu University, Chengdu, China

Molecular recognition of ITIM/ITSM domains with SHP2 and their allosteric effect

In this work, the complete structure of the intact PD-1 tail (ITIM/ITSM peptide) in complex with SHP2 was firstly obtained *via* homologous modelling and molecular docking methods. According to comparative molecular dynamics simulations, the inactive SHP2 remains in a-state conformation with high probability, and has a higher affinity for ITIM/ITSM than active SHP2. In addition, a possible allosteric activation mechanism with C-SH2 as the fulcrum was proposed. The simulation results provide theoretical guidance for structure-based molecular design of novel anticancer drugs.

As featured in:

See Ting Luo *et al.*, *Phys. Chem. Chem. Phys.*, 2024, **26**, 9155.

ROYAL SOCIETY OF CHEMISTRY

rsc.li/pccp

Registered charity number: 207890

PCCP Owner Societies