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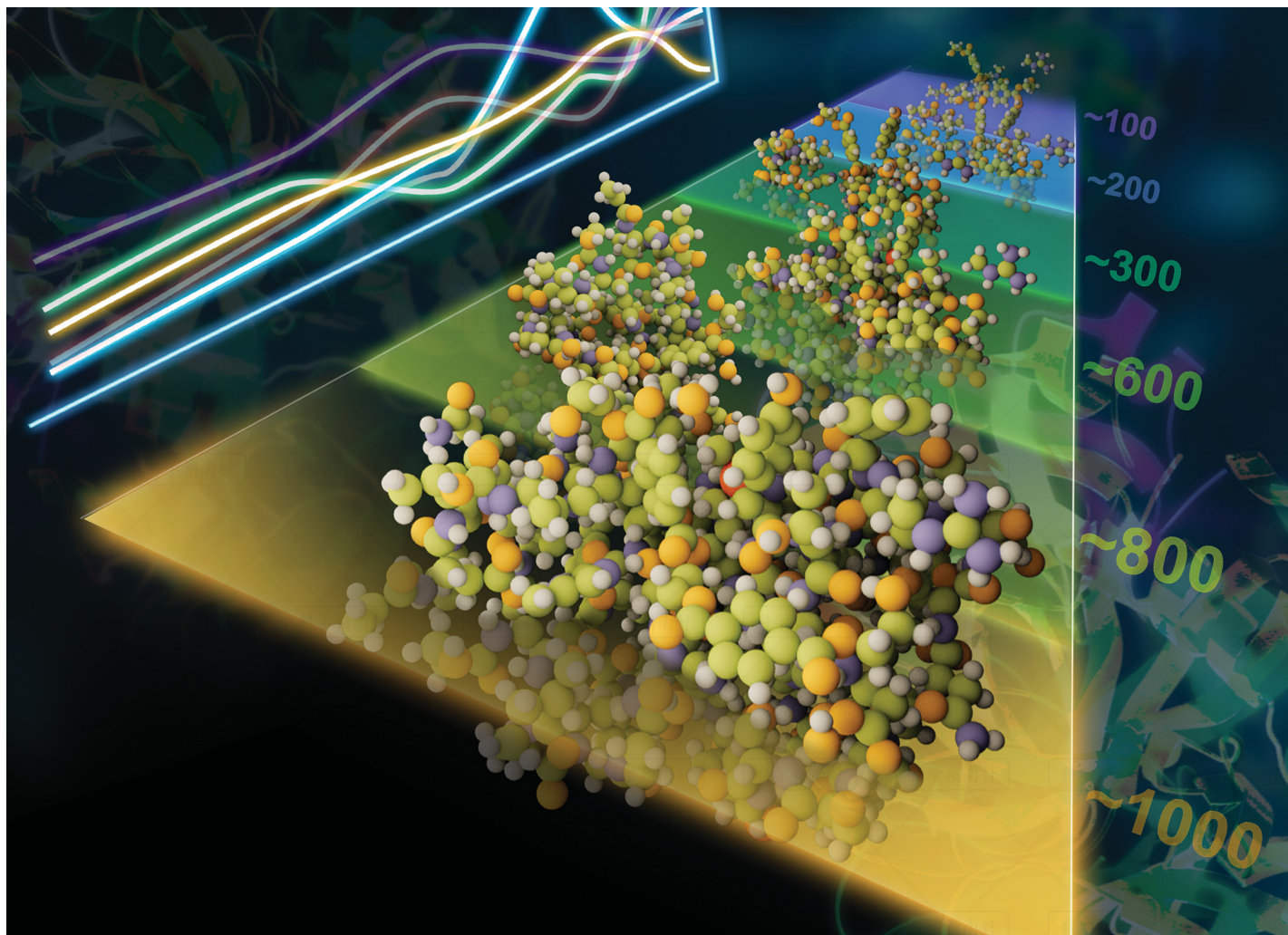
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**Showcasing research from the group of Professor Yanwei Li,
Shandong University, China**

Impacts of QM region sizes and conformation numbers on modelling enzyme reactions: a case study of polyethylene terephthalate hydrolase

This work investigates the convergence behavior of energy barrier and feature parameters influenced by the QM region size and conformation number. Our results show that the convergence behavior can be quite different in different enzyme conformations. Most of the cases show that at least 500 QM atoms are needed. With six conformations considered, the standard deviation of average energy barriers and feature parameters based on multiple conformations with respect to QM region size was decreased.

As featured in:



See Yanwei Li *et al.*,
Phys. Chem. Chem. Phys.,
2023, **25**, 31596.