

- Funding from the United Kingdom's Engineering and Physical Sciences Research Council (EPSRC) (EP/T51780X/1), and Syngenta.
- Computational resources from the UK Materials and Molecular Modelling Hub, which is partially funded by EPSRC (EP/T022213/1, EP/W032260/1 and EP/P020194/1).
- Computational resources provided by Imperial College London's High-Performance Computing Cluster (<http://doi.org/10.14469/hpc/2232>).