

Funding and Computational resource support for this work (including past and continuing):

- Funding support:
 - UK-EP SRC, grant no EP/V010840/1
 - Oxford University Press John Fell Fund
- Computational Resources
 - Marconi 100 supercomputer at CINECA (via PRACE award no. 2021240015)
 - NERSC at Berkeley Lab (via the Molecular Foundry User Program)
 - TACC at UT Austin (via the XSEDE program, award number TG-DMR190070)
 - Summit at Oak Ridge National Lab (via a DOE INCITE program)
 - Local computing resources at the supercomputer ARC, Oxford University.