

[Challenges in large scale quantum mechanical calculations](#)

URL: <http://onlinelibrary.wiley.com/doi/10.1002/wcms.1290/abstract>

Authors: [Ratcliff, Laura](#) / [Mohr, Stephan](#) / [Huhs, Georg](#) / [Deutsch, Thierry](#) / [Masella, Michel](#) / [Genovese, Luigi](#)

Research Lines: [Ab-Initio Electronic Structure Methods](#)

Publication: Wiley Interdisciplinary Reviews: Computational Molecular Science

Volume / Number / Pagination: 7 / 1 / e1290

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

Source URL (retrieved on 10 Mar 2025 - 20:04): <https://www.bsc.es/es/research-and-development/publications/challenges-large-scale-quantum-mechanical-calculations>