

[Complexity Reduction in Density Functional Theory Calculations of Large Systems: System Partitioning and Fragment Embedding](#)

URL: <https://pubs.acs.org/doi/abs/10.1021/acs.jctc.9b01152>

Authors: [Dawson, William](#) / [Mohr, Stephan](#) / [Ratcliff, Laura](#) / [Nakajima, Takahito](#) / [Genovese, Luigi](#)

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

Publication: Complexity Reduction in Density Functional Theory Calculations of Large Systems: System Partitioning and Fragment Embedding

Volume / Number / Pagination: 16 / 5 / 2952-2964

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

Source URL (retrieved on 9 Nov 2024 - 03:11): <https://www.bsc.es/es/research-and-development/publications/complexity-reduction-density-functional-theory-calculations>