

[An efficient implementation of a QM-MM method in SIESTA](#)

URL: <http://www.scopus.com/inward/record.url?eid=2-s2.0-79952190966&partnerID=MN8TOARS>

Authors: [Sanz-Navarro, C.F](#) / [Grima, Rogeli](#) / [Garcia, Alberto](#) / [Bea, E.A.](#) / [Soba,](#) / [Cela, J.M.](#) / [Ordejón, Pablo](#)

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

Publication: An efficient implementation of a QM-MM method in SIESTA

Place Published: Theoretical Chemistry Accounts

Volume / Number / Pagination: 128 / 4 / 825-833

Palabras clave: [Density functional theory](#), [Load balancing](#), [Molecular mechanics](#), [parallelization](#)

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

Source URL (retrieved on 25 Sep 2023 - 09:28): <https://www.bsc.es/es/research-and-development/publications/efficient-implementation-qm-mm-method-siesta>