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## **SIESTA-PEXSI: massively parallel method for efficient and accurate ab initio materials simulation without matrix diagonalization**

**URL:** <https://iopscience.iop.org/article/10.1088/0953-8984/26/30/305503>

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

**Publication:** Journal of Physics: Condensed Matter

**Volume / Number / Pagination:** 26 / 30 / 305503

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**Source URL (retrieved on 10 Mar 2025 - 20:01):** <https://www.bsc.es/es/research-and-development/publications/siesta-pexsi-massively-parallel-method-efficient-and-accurat-0>