

Abstract Submitted
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Spectrum slicing methods to solve the Kohn-Sham problem¹

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— Very large first-principles electronic structure calculations present a challenge as the number of atoms increases owing to the scaling of the eigenvalue problem. We present a spectrum slicing method by which the eigenvalue problem is solved in a divide and conquer fashion. This reduces the cost of quadratic scaling tasks such as orthogonalization in exchange for an increase in the number matrix-vector products. The algorithm is demonstrated on a large system of aluminum atoms in the liquid state.

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