# Large-scale *O*(N) DFT calculations for carbon at high temperature

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Kohn-Sham Density Functional Theory (DFT) implementations based on planewaves have been successfully applied for various materials in the warm dense matter regime. However, the tractable number of particles is rather limited due to the method's $O(N^3)$ scaling and it becomes challenging to employ at high temperatures, where the number of partially occupied states increases significantly. Both problems are addressed with the novel SQDFT code [1], which is a large-scale implementation of the Spectral Quadrature (SQ) method for *O*(N) Kohn-Sham DFT calculations [2,3]. Here, we present extensive benchmark calculations for selected equation of state points for carbon in comparison to the widely-used planewave Kohn-Sham DFT codes VASP [4] and QUANTUM ESPRESSO [5]. Finally, we calculate the Hugoniot curve for carbon at temperatures up to 500 000 K.

## REFERENCES

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