Tungsten modelling from large-scale ab-initio methods

J.J. Gutiérrez Moreno[1], S. Mohr[1,2], M. Mantsinen[1,3]

[1] *Barcelona Supercomputing Center (BSC), C/ Jordi Girona 31, 08034 Barcelona, Spain*

[2] *Nextmol (Bytelab Solutions SL), C/ Roc Boronat 117, 08018 Barcelona, Spain*

[3] *ICREA, Pg. Lluís Companys 23, 08034 Barcelona, Spain*

Tungsten is one of the best plasma-facing candidate materials due to its strength, high stability and excellent thermal conductivity. However, defects produced by neutron irradiation may have detrimental effects on its structure and affect its properties. Ab initio density functional theory (DFT) calculations have been typically used to elucidate the characteristics of the smallest defects in a wide range of materials with very high accuracy. Unfortunately, the computational cost in standard DFT calculations is proportional to the cube of the number of electrons, limiting accessible systems to a few hundreds of atoms.

This work shows that DFT calculations for large systems are possible with the so-called linear scaling (LS) algorithms, meaning that doubling the number of atoms in a system leads to a computation time only twice as large. The LS version of the wavelet-based BigDFT code is used to model defective metallic systems with thousands of atoms, yielding results comparable to conventional cubic-scaling DFT.[1] Our electronic structure models of tungsten metal are in good agreement with plane-wave DFT and are successfully compared against the experimental features in tungsten's photoelectron spectrum.[2, 3] These calculations show the possibility of addressing the challenge of simulating realistic defective and disordered mixed-metal alloys with ab-initio accuracy, which can be used as a guide for the development of new materials for fusion applications.

References

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