

Predicting temperature-dependent elastic constants for ultra-high temperature ceramics

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Language Undefined

Description:

Proyecto asignado a través de la [Red Española de Supercomputación](#) [2].

Ultra-high temperature ceramics, UHTCs, are key components of materials used in extreme conditions for aerospace applications. However, the characterisation of these materials at working conditions is extremely expensive and there are few laboratories over the world with the required facilities for that task. Although elastic constant at 0 K are calculated routinely by first principles, temperature-dependent elastic constant calculations are still a difficult challenge because of the lack of well established approaches and the high computational cost of these methodologies. In this activity, we strive to calculate the temperature-dependent elastic constants of UHTC materials.

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Links

[1] <http://www.us.es/>

[2] <https://www.res.es/>