

Abstract Submitted  
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**Ab-initio melting curve of titanium** VINCENT STUTZMANN, JOHANN BOUCHET, FRANCOIS BOTTIN, None — Thermodynamical properties of titanium are of great interest for aerospace and aviation industries and many studies are done in order to understand its behaviour under pressure (P) and temperature (T) : phase transitions at low T, melting curve at high T and P. In this work we compute the first *ab-initio* melting curve of titanium. This one is obtained with the ABINIT package using DFT, in the GGA approximation, and in the framework of the projector augmented wave method (PAW). At first, we perform ground state calculations and study the five allotropic phases of titanium. Two PAW atomic data are generated with two different cutoff radius. The larger one gives results near previous *ab-initio* calculations, whereas the smaller one gives results near all electron calculation. Using the second PAW atomic data and performing *ab-initio* molecular dynamic simulations, we then compute the melting curve of titanium with three different methods. Results show relevance of our calculations, but also discrepancies with experimental data.

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None

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