

Abstract Submitted
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Fully *ab initio* melting curve of aluminium up to 350 GPa JOHANN BOUCHET, FRANCOIS BOTTIN, GERALD JOMARD, Commissariat a l'Energie Atomique — We performed *ab initio* molecular dynamics simulations to compute the melting curve of aluminium. Both the two-phase (TP) and heat-until melt (HUM) methods have been considered. The former describes an heterogeneous mechanism with a well-defined melting temperature T_m . On the other hand, in the HUM the crystal melts homogeneously and can be overheated above T_m . The limit of superheating is the critical temperature T_{LS} . Calculations are carried out in the NVT ensemble up to 350 GPa with supercells of different sizes. For each method, we present the convergence of the melting curves as a function of the number of atoms, and compare our results with previous calculations and experiments. We also discuss the evolution of the degree of overheating with respect to the pressure. At last, by means of NPT simulations we also compute volume change on melting, which is in good agreement with previous free energy calculations.

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