

# Multiscale approaches based on ab-initio calculations

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Recent developments are promising to make possible the modelling of mechanical properties of materials across length scales, using ab-initio calculations. One such approach which holds the promise of wide applicability involves the use of an orbital-free, real-space formulation of density functional theory, which should provide a natural way for applying arbitrary boundary conditions. A different approach relies on a sophisticated continuum formulation of the behavior of dislocations, in the spirit of the Peierls-Nabarro theory, which can be solved variationally. A key ingredient in this approach is the generalized stacking fault energy surface, which can capture the effect of changes in the chemical composition of a solid. I will review these developments and discuss their possible applications in large-scale simulations of the mechanical response of solids based exclusively on ab-initio calculations.