1. First-principles investigations of solids

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Solving Schrödinger equation: $\left[-\frac{1}{2}\nabla^2 + V(r) + \mu_{xc}(r)\right] \Psi_i^k(r) = \varepsilon_i^k \Psi_i^k(r)$

➔ phase stability, elastic properties,
microstructure, precipitation, impurity distribution