

Simulations of Aluminum-Silicon alloys

As the first step of modeling the tribological phenomena at the aluminum engine surface, quantum-mechanical total-energy pseudopotential calculations are performed on Al-Si alloys. Some approximation parameters involved in the total-energy calculations such as **k** points, energy cutoff, and pseudopotential types are studied and selected to get more reasonable results as well as higher calculation efficiency. Pure Aluminum and some ordered Al-Si alloys (12.5% at. Si and 25% at. Si) are chosen to do single point energy calculations as a function of volume. After fitting the EOS, some solid properties such as lattice parameter and bulk modulus have been calculated. All the information provides us a basis to construct a good force field to model the complex tribological systems without detailed experimental data on these phenomena.