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Ab Initio Study of the Effect of Solute Atoms on Stacking Fault Energy in Aluminum YUE QI, RAJA MISHRA, GM R&D Center — The stacking fault energy (SFE) in binary and ternary alloys of Al with common alloying elements was studied using density function theory. Among these alloying elements, Fe further increases the SFE and Ge reduces the SFE of Al. The elements increasing the directional inhomogeneity in the electronic charge distribution of the FCC structure correlates with the increasing SFE. The maximum value of charge difference on the fault plane, Max($\Delta\rho$), is used to characterize how much electron has been redistributed due to the stacking fault formation, and the SFE monotonically increases with Max($\Delta\rho$).

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