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Surface Relaxation of Aluminum

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We performed a total energy calculation of clean aluminum surfaces of three low indices based on a density functional theory with a local density approximation, using the Ceperly-Alder exchange correlation parametrized by Perdew and Zunger. Pseudopotentials were generated for Al of which the plane wave cut-off was 15*Ry*. We used Gaussian broadening of a Fermi level to accelerate the convergence of our calculation with the Gaussian energy smearing parameter of 0.005*Ry*.

First, we determine the lattice constant of the aluminum of an face-centered-cubic structure to be 3.96 Å which is comparable to the experimental data of 4.05 Å. The cohesive energy of 4.20eV/atom and the bulk modulus of $0.775\times 10^{12} dyne/cm^2$ are also comparable to the experimental values of 3.39eV/atom and $0.722\times 10^{12} dyne/cm^2$, respectively. Then we investigated the surface relaxation of (100), (110) and (111) surfaces using a 9-layer slab separated by 6-layer thick vacuum. The results are consistent with the existing experimental results.