> Total_energy (RELAX) =  -15.8529325684 Ry

> Total Energy (natoms-64) [BULK-optimization] =  -506.8966179159 Ry

> Total Energy (natoms-64) [SURFACE-optimization-100]= -502.69885972 Ry
(convergence has been achieved in  23 iterations)

> Total Energy (natoms-64) [SURFACE-optimization-111]= -500.35268267 Ry
(convergence NOT achieved after 100 iterations)

> Surface energy = (1/2) * (E_slab - N * E_bulk) = 0.5*(-502.69885972 +
506.8966179159) Ry = 2.09887909795 Ry