

# tsmear vs Etot and Lattice Constant

tsmear (K)

100 200 300 400 500 600 700

-3.6748e1

-0.00005

-0.00010

-0.00015

-0.00020

-0.00025

-0.00030

-0.00035

-0.00040

10.528

10.526

10.524

10.522

10.520

10.518

10.516

Lattice Constant (Bohr)

Etot (hartree)

0.01

0.02

0.03

0.04

0.05

0.06

tsmear (eV)

