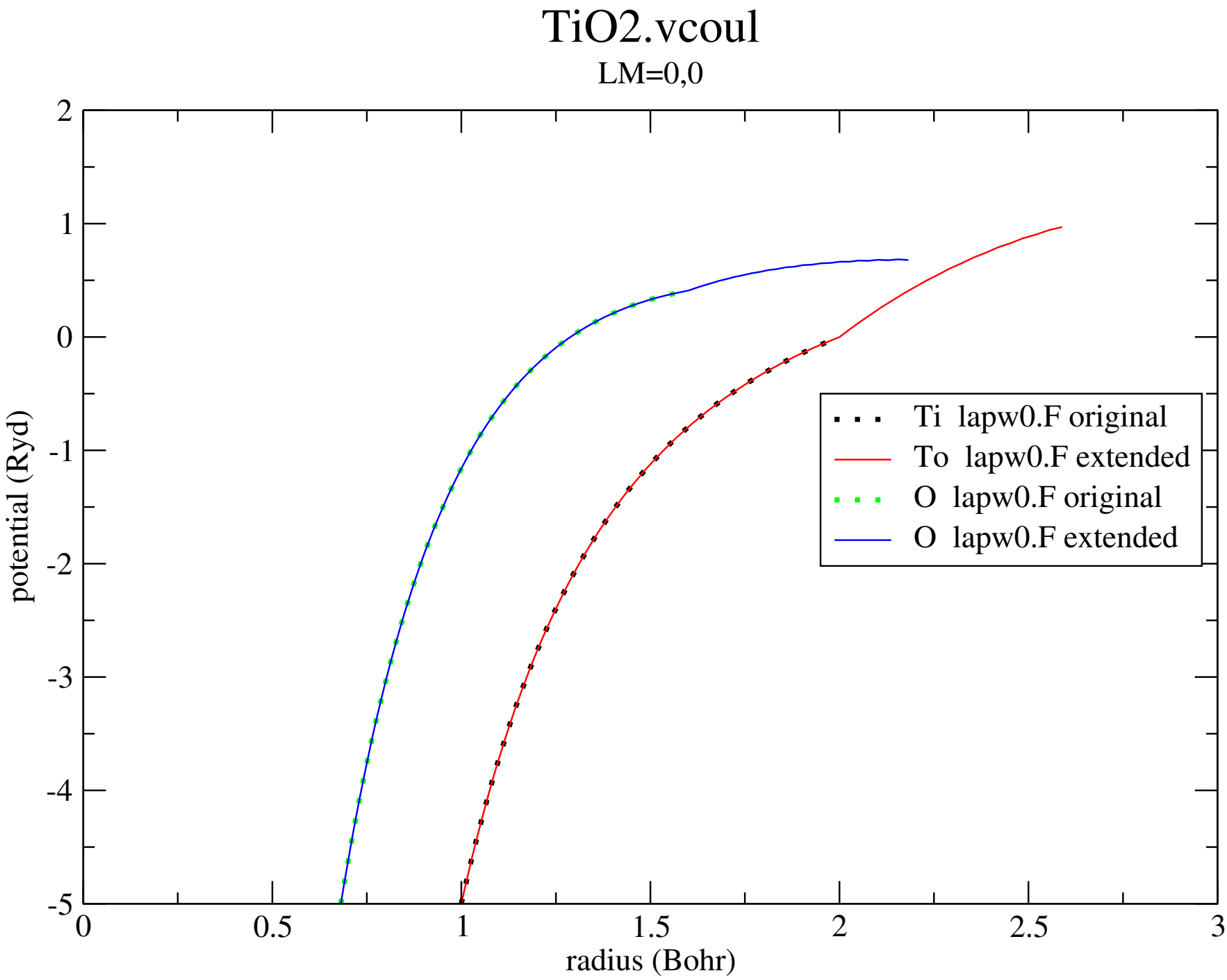
TiO2.vcoul
LM=0,0
potential (Ryd)
radius (Bohr)
2
1
0
-1
-2
-3
-4
-5
0
0.5
1
1.5
2
2.5
3
Ti lapw0.F original
To lapw0.F extended
O lapw0.F original
O lapw0.F extended