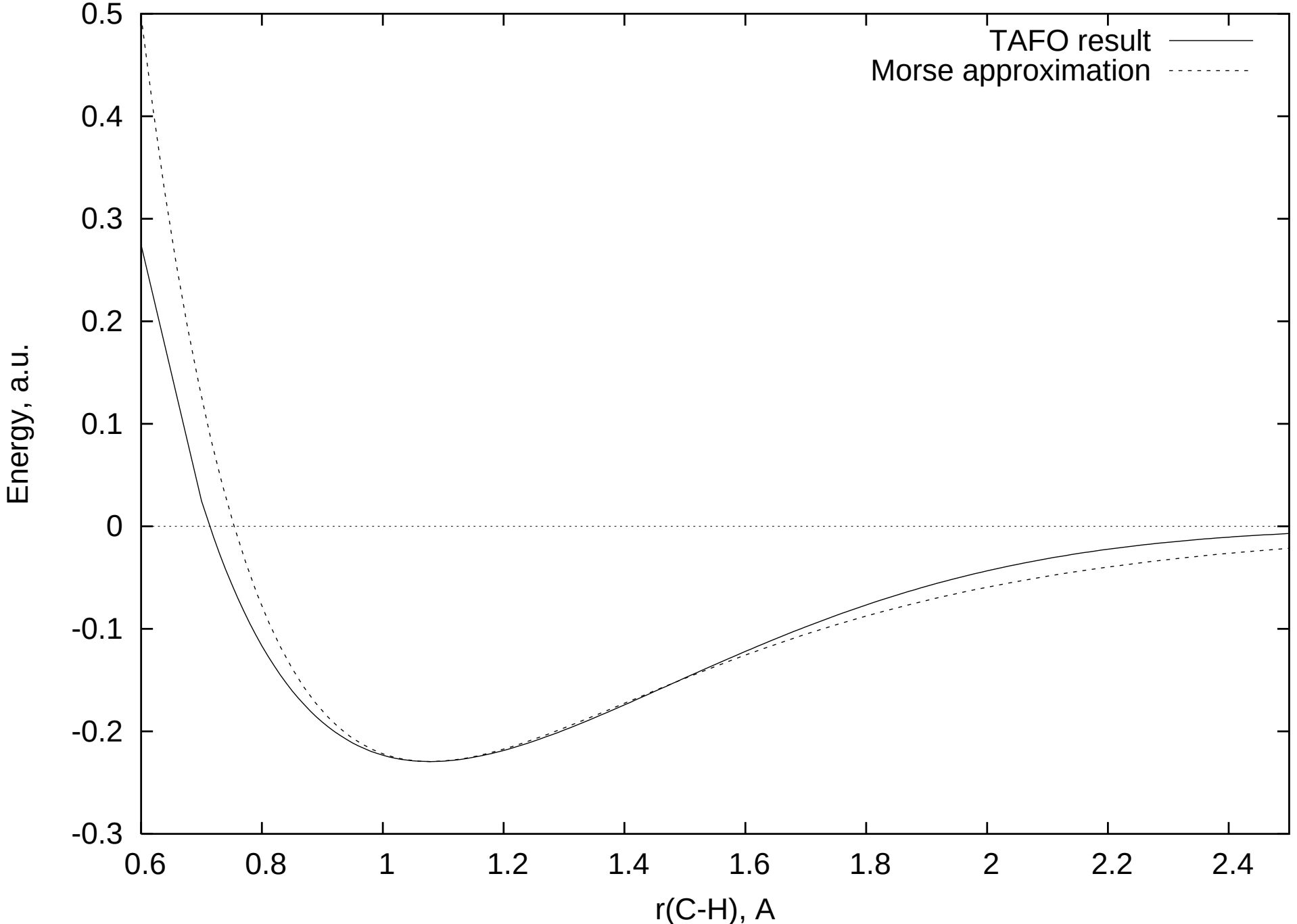
TAFO result
Morse approximation
Energy, a.u.
r(C-H), A
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0.6
0.8
1
1.2
1.4
1.6
1.8
2
2.2
2.4