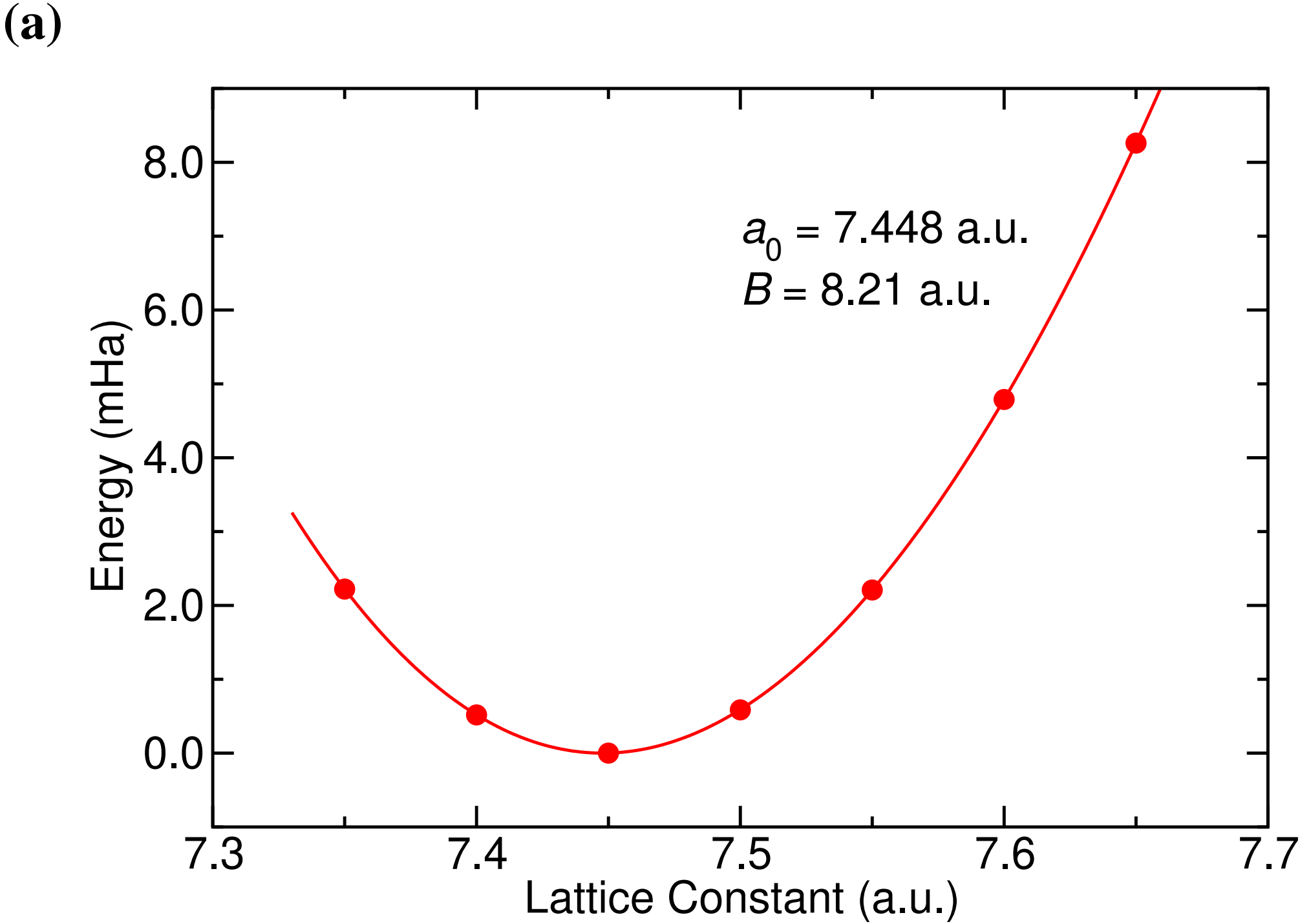
(a)
8.0
6.0
4.0
2.0
0.0
Energy (mHa)
a_0 = 7.448 a.u.
B = 8.21 a.u.
7.3
7.4
7.5
7.6
7.7
Lattice Constant (a.u.)